

FILE 'REGISTRY' ENTERED AT 08:12:17 ON 01 AUG 2002

L1 673500 S 4/SZS
 L2 205560 S 4/SZ
 L3 3789863 S 5/SZ
 L4 26014 S L2 AND L3
 L5 26014 S L1 AND L4
 L6 8078 S L5 AND C4/EA
 L7 0 S L6 AND C4-C5/EA
 L8 0 S L5 AND C4-C5/EA
 L9 112 S L5 AND HG/ELS
 L10 62 S L9 AND S/ELS
 L11 22 S L10 AND (ION OR COMPLEX OR CATION OR RADICAL)
 L12 0 S L9 AND (HG/ELS NOT HG/REL)
 L13 221 S C5/EA AND (HG/ELS NOT HG/REL)
 L14 221 S L13 AND (1 OR 2)/NRRS
 L15 30913 S C5/EA AND (S/ELS NOT S/REL)
 L16 19 S L14 AND L15
 L17 31 S THIOMERCURI/BI
 L18 280 S MERCURITHIO? OR THIOMERCUR?
 L19 19 S PENTAMERCUR?
 L20 143 S TETRAMERCUR?
 L21 205 S TRIMERCUR?
 L22 1 S BIMERCUR?
 L23 925 S DIMERCUR?
 L24 0 S L13 AND (L17 OR L18 OR L19 OR L20 OR L21 OR L22 OR L23)
 SAVE L1-24 TODAY/L
 L25 54127 S CYCLOBUTA?
 L26 444088 S CYCLOPENTA?
 L27 324634 S (L2 OR L3) AND (C5 OR C4)/EA
 L28 24755 S L27 AND L25
 L29 93607 S L27 AND L26
 L30 4012 S L27 AND (SC OR TI OR V OR CR OR FE OR CO OR NI OR CU OR ZN OR Y OR ZR OR NB OR
 MO OR TC OR RU OR RB OR PD OR AG OR CD)/ELS
 L31 855 S L30 NOT (SC OR TI OR V OR CR OR FE OR CO OR NI OR CU OR ZN OR Y OR ZR OR NB OR MO
 OR TC OR RU OR RB OR PD OR AG OR CD)/REL
 L32 368 S (L28 OR L29) AND L31
 L33 116 S L27 AND (LA OR HF OR TA OR W OR RE OR OS OR IR OR PT OR AU OR HG)
 L34 1622 S L27 AND (LA OR HF OR TA OR W OR RE OR OS OR IR OR PT OR AU OR HG)/ELS
 L35 1656 S (L33 OR L34)
 L36 932 S L35 NOT (LA OR HF OR TA OR W OR RE OR OS OR IR OR PT OR AU OR HG)/REL
 L37 564 S (L28 OR L29) AND L36
 L38 1784 S L31 OR L36
 L39 932 S L32 OR L37

FILE 'HCAPLUS' ENTERED AT 09:17:13 ON 01 AUG 2002

L40 1469 S L38
 L41 613 S L39

FILE 'REGISTRY' ENTERED AT 09:17:31 ON 01 AUG 2002

L42 787 S L40 AND (ION OR COMPLEX OR CATION OR RADICAL)
 L43 503 S L41 AND (ION OR COMPLEX OR CATION OR RADICAL)
 L44 107 S L42 AND (HG/ELS NOT HG/REL)
 L45 77 S L43 AND (HG/ELS NOT HG/REL)
 L46 31 S L43 AND (S/ELS NOT S/REL)
 L47 53 S L42 AND (S/ELS NOT S/REL)
 L48 107 S L42 AND (HG/ELS NOT HG/REL)
 L49 6 S L45 AND L46
 L50 12 S L47 AND L48

L51 6 S L50 NOT L49
 L52 787 S L38 AND (ION OR COMPLEX OR CATION OR RADICAL)
 L53 150 S L52 AND (L25 OR L2 OR C4/EA)
 L54 643 S L52 AND (L3 OR L26 OR C5/EA)
 L55 6 S L53 AND L54
 L56 1404 S L38 AND (L3 OR L26 OR C5/EA)
 L57 420 S L38 AND (L25 OR L2 OR C4/EA)
 L58 40 S L56 AND L57
 L59 221 S L56 AND HG/ELS
 L60 221 S L59 NOT HG/REL
 L61 19 S L60 AND S/ELS
 L62 150 S L57 AND (ION OR COMPLEX OR CATION OR RADICAL)
 L63 0 S L57 AND POLAR#####

FILE 'HCAPLUS' ENTERED AT 09:38:02 ON 01 AUG 2002

L64 8 S L55 OR (L49 OR L50 OR L51)
 L65 17 S L58
 L66 4 S L61
 L67 135 S L62
 L68 155 S L60
 L69 255 S L57
 L70 1315 S L56
 L71 1469 S L38
 L72 13 S L65 NOT (L64 OR L66)

FILE 'SCISEARCH' ENTERED AT 09:41:12 ON 01 AUG 2002

L73 1 S "KOLOBOVA N E, 1986, P711, IZV AKAD NAUK SSSR K"/RE

FILE 'HCAPLUS' ENTERED AT 09:44:18 ON 01 AUG 2002

L74 4 S L65 AND (L64 OR L66)

FILE 'REGISTRY' ENTERED AT 09:46:15 ON 01 AUG 2002

L75 1 S MERCURY/CN

FILE 'HCAPLUS' ENTERED AT 09:46:16 ON 01 AUG 2002

L76 9 S L75 AND (L67 OR L68 OR L69 OR L70 OR L71)
 L77 1 S L67 AND L68 AND L69 AND L70 AND L71
 L78 1 S L67 AND L68 AND L69 AND L70
 L79 1 S L67 AND L68 AND L70 AND L71
 L80 73 S L67 AND L69 AND L70 AND L71
 L81 3 S L68 AND L69 AND L70 AND L71
 L82 101 S L69 AND L70 AND L71
 L83 1 S L67 AND L68 AND L69
 L84 1 S L67 AND L68 AND L70
 L85 1 S L67 AND L68 AND L71
 L86 3 S L68 AND L70 AND L69
 L87 155 S L68 AND L70 AND L71
 L88 101 S L69 AND L70 AND L71
 L89 73 S L67 AND L70 AND L71
 L90 135 S L67 AND L69 AND L71
 L91 3 S ((L77 OR L78 OR L79) OR L81 OR (L83 OR L84 OR L85 OR L86)) NOT (L76 OR L65)
 L92 315 S (L80 OR L82 OR (L87 OR L88 OR L89 OR L90))
 L93 288 S L92 NOT ((L77 OR L78 OR L79) OR L81 OR (L83 OR L84 OR L85 OR L86) OR L76 OR L65)
 L94 0 S L93 AND ROTOR
 L95 0 S L93 AND MOTOR
 L96 1 S L93 AND MICRO#####
 L97 0 S L93 AND MEMS

L98 0 S L93 AND MICROELEC?
 L99 0 S L93 AND MICROMECH?
 L100 0 S L93 AND NANO#####
 L101 17 S L58
 L102 8 S C07F/IC
 L103 845 S C07F007-12/IC
 L104 2423 S C07F007-08/IC
 L105 278 S (C07F007-14/IC OR C07F007-16/IC)
 L106 9133 S C07F007?/IC
 L107 2 S L93 AND (L102 OR L103 OR L104 OR L105 OR L106)
 L108 1 S L93 AND DIPOLAR?
 L109 18 S L93 AND (POLAR? OR ?CHARG?)
 L110 19 S L93 AND (?POLAR? OR ?CHARG?)
 L111 317 S L108 OR L107 OR L92 OR (L77 OR L78 OR L79) OR L81 OR (L83 OR L84 OR L85 OR L86) OR L76 OR L65
 L112 18 S L110 NOT (L107 OR L108)
 L113 267 S L93 NOT (L107 OR L108 OR L110)
 L114 7 S L113 AND ROTAT?
 L115 260 S L113 NOT L114
 L116 4 S (105557-66-2/BI OR 105557-66-2P/BI OR 105557-67-3/BI OR 105557-67-3P/BI OR)

FILE 'REGISTRY' ENTERED AT 10:12:34 ON 01 AUG 2002

L117 19 S L115 AND HG/ELS AND S/ELS
 L118 5357 S (HG/ELS AND S/ELS AND C/ELS) NOT (HG/REL OR S/REL)

FILE 'HCAPLUS' ENTERED AT 10:13:56 ON 01 AUG 2002

L119 10 S L118 AND L115
 L120 11 S L115 AND TRANSITION METAL
 L121 1 S TRANSITION METAL AND ROTOR AND CYCLOPENT? AND CYCLOBUT?
 L122 4 S TRANSITION METAL AND ROTOR AND (CYCLOPENT? OR CYCLOBUT?)
 SEL RN
 L123 3 S L122 AND (12108-04-2/BI OR 14808-60-7/BI OR 1558-25-4/BI OR 368884-91-7/BI OR 368884-92-8/BI OR 65209-16-7/BI OR 65209-17-8/BI OR 7439-97-6/BI OR 7440-62-2/BI)
 L124 1 S L122 NOT L123
 L125 3 S ROTOR AND CYCLOPENT? AND CYCLOBUT?
 SEL RN
 L126 3 S L125 AND (110-83-8/BI OR 142-29-0/BI OR 822-35-5/BI OR 110-82-7/BI OR)
 L127 59 S DIPOL? AND CYCLOPENT? AND CYCLOBUT?
 L128 1 S TRANSITION METAL AND L127
 L129 4 S METAL AND L127
 SEL RN
 L130 3 S L129 AND (1191-95-3/BI OR 122093-43-0/BI OR 14333-24-5/BI OR 14808-60-7/BI OR)

FILE 'REGISTRY, MARPAT, MARPATPREV, CAPLUS' ENTERED AT 10:57:14 ON 01 AUG 2002

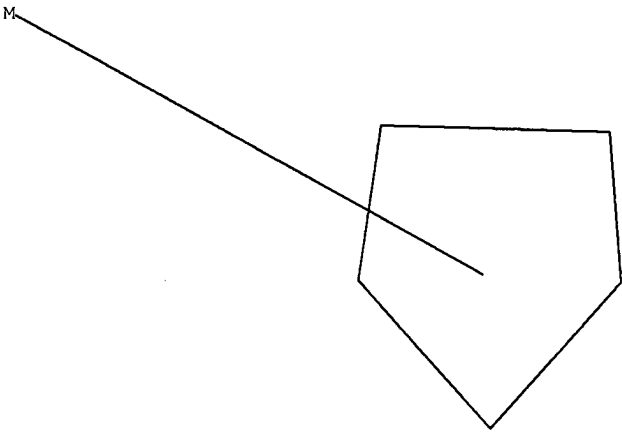
L15 STRUCTURE UPLOADED
L16 STRUCTURE UPLOADED
L17 1 SEA SSS SAM L15
L18 0 SEA SSS SAM L15
L19 0 SEA SSS SAM L16
L20 1 SEA SSS SAM L16

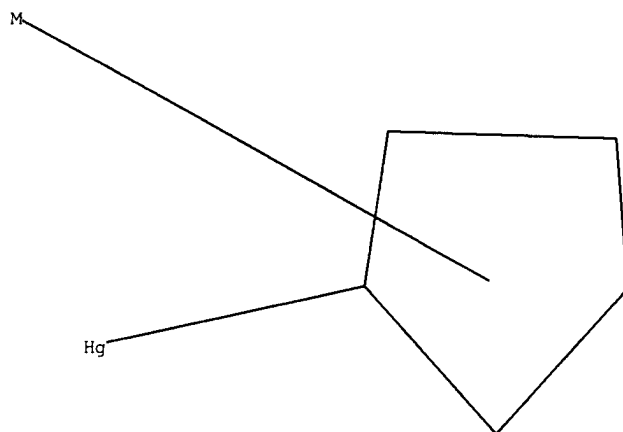
FILE 'MARPAT' ENTERED AT 10:58:30 ON 01 AUG 2002

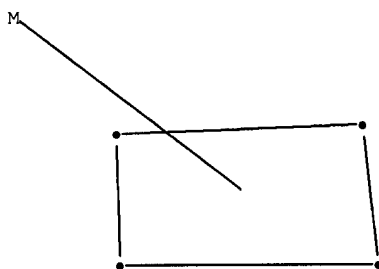
L21 1 SEA SSS FUL L15
L22 13 SEA SSS FUL L16
L23 14 S (L21 OR L22)

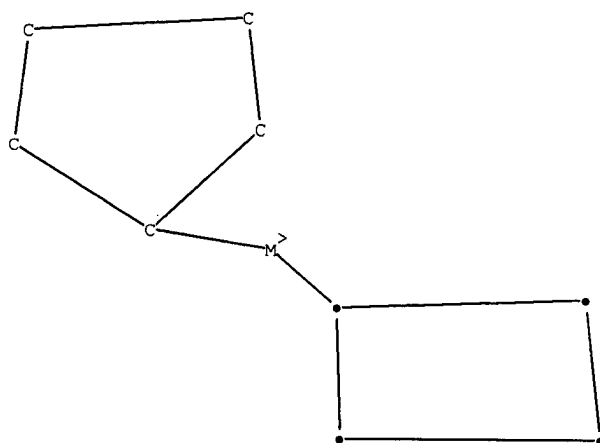
FILE 'REGISTRY, MARPAT, MARPATPREV, CAPLUS' ENTERED AT 11:14:35 ON 01 AUG 2002

L30 STRUCTURE UPLOADED
L31 0 SEA SSS SAM L30
L32 0 SEA SSS SAM L30
L33 0 SEA SSS FUL L30
L34 2 SEA SSS FUL L30
L35 0 SEA SSS FUL L30
L36 0 S L33
SET DUPORDER FILE
L37 2 DUP REM L35 L34 L36 (0 DUPLICATES REMOVED)
 ANSWERS '1-2' FROM FILE MARPAT









L116 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2002 ACS

AN 1986:627025 HCAPLUS

DN 105:227025

TI Nonionic and anionic surface-active ferrocene derivatives

IN Haage, Klaus; Weiland, Bernd; Sonnek, Georg; Reinheckel, Heinz;
Rybinskaya, M. I.; Kaganovich, V. S.; Krivykh, V. V.

PA Akademie der Wissenschaften der DDR, Ger. Dem. Rep.

SO Ger. (East), 6 pp.

CODEN: GEXXA8

DT Patent

LA German

FAN.CNT 1

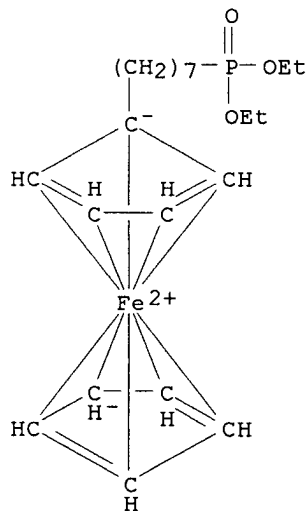
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DD 234274	A1	19860326	DD 1984-271521	19841227

AB R1(CR2R3)nX [R1 = (substituted) ferrocenyl; R2, R3 = H, alkyl; n = 1-20; X = hydrophilic group], useful as nonionic and anionic surface-active agents, are prepd. Thus, ethylene oxide was fed over 2.0 g 4-ferrocenyl-1-butanol for 1 h at 80-100.degree. under N and in the presence of BF3.OEt2 to give 5.9 g R1(CH2)4(OCH2CH2)12OH (R1 = ferrocenyl), which in surface tension redn. tests showed .sigma.CMC = 46.0 mN/m.

IT **105557-66-2P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and sapon. of, monoester from)

RN 105557-66-2 HCAPLUS

CN Ferrocene, [7-(diethoxyphosphinyl)heptyl]- (9CI) (CA INDEX NAME)



L114 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2002 ACS

AN 1981:471407 HCAPLUS

DN 95:71407

TI Chromium squarates: $\text{Cr}(\text{C4O4})(\text{OH}) \cdot 3\text{H}_2\text{O}$ and $\text{Cr}(\text{C4O4})_{3/2} \cdot 7\text{H}_2\text{O}$

AU Chesick, John P.; Doany, Fuad

CS Dep. Chem., Haverford Coll., Haverford, PA, 19041, USA

SO Acta Crystallogr., Sect. B (1981), B37(5), 1076-9

CODEN: ACBCAR; ISSN: 0567-7408

DT Journal

LA English

AB $\text{Cr}(\text{C4O4})(\text{OH}) \cdot 3\text{H}_2\text{O}$ is triclinic, space group $P\bar{1}$, with a 7.490(2), b 7.540(3), c 8.120(3) Å, α 106.28(2)°, β 95.16(2)°, and γ 113.86(2)°. $d(\text{exptl.}) = 1.97$ and $d(\text{calcd.}) = 1.99$ for $Z = 2$; $R = 0.045$ for 922 reflections. Two $\text{Cr}(\text{OH})(\text{C4O4})$ units, related by a center of symmetry, exist as dimers. The Cr pairs are joined by 2 μ -hydroxo bridges and by 2 C4O4^{2-} ions acting as bridging groups through adjacent O atoms. The O atoms of 2 H_2O mols. complete the octahedral coordination of each Cr ion. H bonds connect the dimeric units to each other and to the one remaining water mol. $\text{Cr}(\text{C4O4})_{3/2} \cdot 7\text{H}_2\text{O}$ is monoclinic, space group $C2/c$, with a 14.878(5), b 15.434(3), c 11.500(3) Å, and β 112.33(6)°. $d(\text{exptl.}) = 1.89$ and $d(\text{calcd.}) = 1.88$ for $Z = 8$. $R = 0.044$ for 1956 reflections. One complete square ion exists in the asym. unit, and another half squarate exists in the asym. unit with 4 atoms on a 2-fold rotation axis. The hexaaquachromium(III) ion is H bonded to the squarate ions and to the remaining H_2O mol. in the asym. unit.

IT 77964-95-5

RL: PRP (Properties)

(crystal structure of)

RN 77964-95-5 HCAPLUS

CN Chromium(3+), hexaaqua-, (OC-6-11)-, salt with 3,4-dihydroxy-3-cyclobutene-1,2-dione (2:3), monohydrate (9CI) (CA INDEX NAME)

CM 1

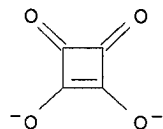
CRN 77964-94-4

CMF C4 O4 . 2/3 Cr H12 O6

CM 2

CRN 28737-40-8

CMF C4 O4



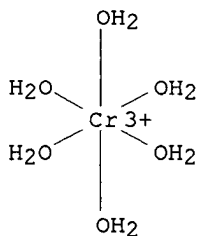
CM 3

CRN 14873-01-9

CMF Cr H12 O6

CCI CCS

CDES 7:OC-6-11



L112 ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2002 ACS

AN 1979:523215 HCAPLUS

DN 91:123215

TI CNDO/2 study of the isoelectronic series of complexes
dicarbonyl(dinitrogen)- and dicarbonyl-.eta.-benzenechromium,
-.eta.-cyclopentadienylmanganese, -.eta.-cyclobutadieneiron, and
-trimethylenemethaneiron obtained by the matrix isolation technique

AU Fitzpatrick, Noel J.; Rest, Antony J.; Taylor, David J.

CS Dep. Chem., Univ. Coll., Dublin, Ire.

SO J. Chem. Soc., Dalton Trans. (1979), (2), 351-4

CODEN: JCDTBI; ISSN: 0300-9246

DT Journal

LA English

AB The electronic structure of the isoelectronic series of title complexes
ML(CO)₂(N₂) and ML(CO)₂ [ML = Cr(.eta.-C₆H₆), Mn(.eta.-C₅H₅),
Fe(.eta.-C₄H₄), Fe[C(CH₂)₃]] was studied within a CNDO/2 formalism, using
both exptl. and std. geometries. The computed trends for CO and N₂ bond
strengths in the complexes, as measured by Wiberg indexes, **charge**
distributions, and orbital populations, correlate well with exptl. CO and
N₂ stretching frequencies and energy-factored stretching force consts.,
i.e. Cr < Mn < Fe, and ML(CO)₂ < ML(CO)₂(N₂) < ML(CO)₃. The computed
total energies of ML(CO)₂ suggest that in all cases a tilted geometry is
preferred, i.e. the plane of the cyclic ligand L is not perpendicular to
the M(CO)₂ plane. CNDO/2 calcns. on Fe[C(CH₂)₃](CO)₃ show that it fits in
well with other ML(CO)₃ complexes.

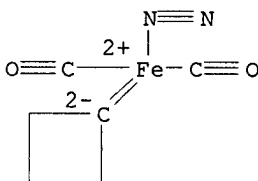
IT 71307-83-0 71307-84-1 71307-85-2

RL: PRP (Properties)

(electronic structure and total energy of, CNDO/2 calcns. of)

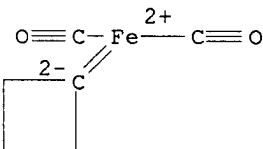
RN 71307-83-0 HCAPLUS

CN Iron, dicarbonylcyclobutylidene(dinitrogen)- (9CI) (CA INDEX NAME)



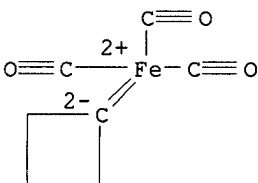
RN 71307-84-1 HCAPLUS

CN Iron, dicarbonylcyclobutylidene- (9CI) (CA INDEX NAME)



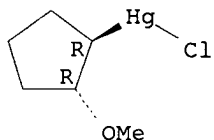
RN 71307-85-2 HCAPLUS

CN Iron, tricarbonylcyclobutylidene- (9CI) (CA INDEX NAME)



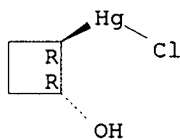
L91 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2002 ACS
 AN 1973:442638 HCAPLUS
 DN 79:42638
 TI Oxymercuration of cycloalkenes
 AU Waters, William L.; Traylor, Teddy G.; Factor, Arnold
 CS Dep. Chem., Univ. Montana, Missoula, Mont., USA
 SO J. Org. Chem. (1973), 38(13), 2306-9
 CODEN: JOCEAH
 DT Journal
 LA English
 AB Hydroxymercuration and methoxymercuration of the 8 stable unsubstituted C4-9 cycloalkenes to give .beta.-hydroxymercurials and .beta.-methoxymercurials, resp. whose configurations were assigned by near-ir hydroxy and NMR methoxy shift measurements. Whereas the 6 cis-cycloalkenes underwent clean trans addn., both trans-cyclooctene and trans-cyclononene reacted in an exclusively cis fashion. The tendency of an olefin to oxymercureate via a trans mechanism is directly, related to its ability to form the normal anti transition state; if for either steric or twist-strain reasons this transition state is unfavorable, cis addn. will prevail.
 IT 29581-86-0P 39837-13-3P 39837-14-4P
 39849-94-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 29581-86-0 HCAPLUS
 CN Mercury, chloro(2-methoxycyclopentyl)-, trans- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.



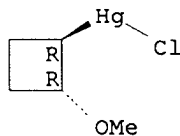
RN 39837-13-3 HCAPLUS
 CN Mercury, chloro(2-hydroxycyclobutyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 39837-14-4 HCAPLUS
 CN Mercury, chloro(2-methoxycyclobutyl)-, trans- (9CI) (CA INDEX NAME)

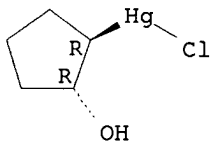
Relative stereochemistry.



RN 39849-94-0 HCAPLUS

CN Mercury, chloro(2-hydroxycyclopentyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L116 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2002 ACS

AN 1986:626908 HCAPLUS

DN 105:226908

TI Synthesis of (.eta.5-cyclopentadienyl)-.eta.1-(2,4-diphenyl-3-thioxo-1-cyclobutenyl)dicarbonyliron and its reactions with Group VI metal carbonyls

AU Kolobova, N. E.; Rozantseva, T. V.

CS Inst. Elementoorg. Soedin. im. Nesmeyanova, Moscow, USSR

SO Izv. Akad. Nauk SSSR, Ser. Khim. (1986), (3), 711-12

CODEN: IASKA6; ISSN: 0002-3353

DT Journal

LA Russian

OS CASREACT 105:226908

AB The title complex (I, X = S) was prepd. by reaction of I (X = O) with P4S10 in THF. The reactions of I (X = S) with M(CO)5.cntdot.THF (M = Mo, W) gave binuclear complexes.

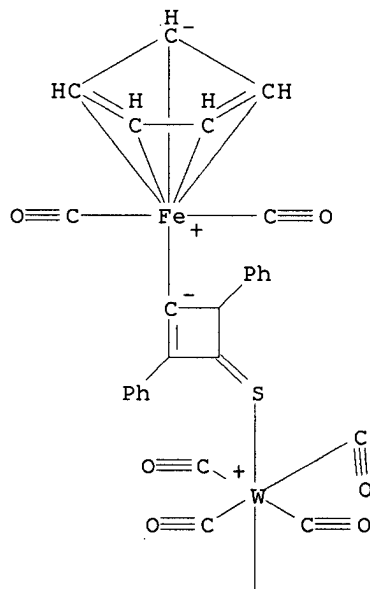
IT 105557-67-3P 105557-68-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 105557-67-3 HCAPLUS

CN Tungsten, pentacarbonyl[dicarbonyl(.eta.5-2,4-cyclopentadien-1-yl)iron][.mu.-(2,4-diphenyl-3-thioxo-1-cyclobuten-1-yl-C:S)]- (9CI) (CA INDEX NAME)

PAGE 1-A

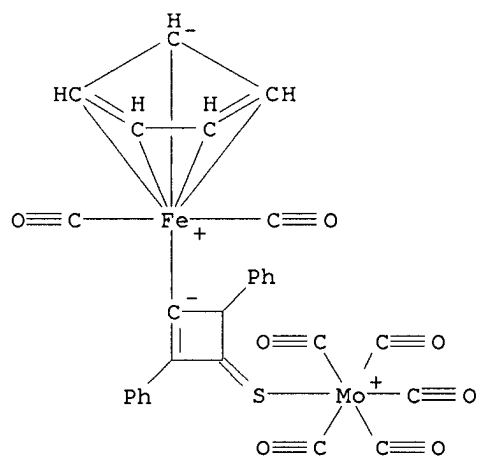


PAGE 2-A

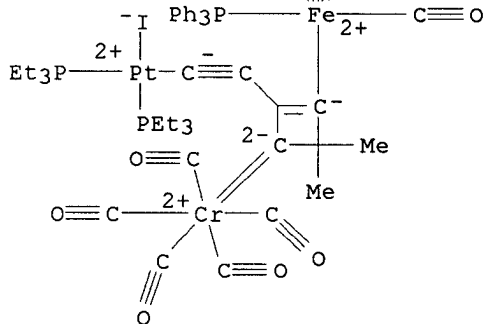


RN 105557-68-4 HCAPLUS

CN Molybdenum, pentacarbonyl[dicarbonyl(.eta.5-2,4-cyclopentadien-1-yl)iron][.mu.-(2,4-diphenyl-3-thioxo-1-cyclobuten-1-yl-C:S)]- (9CI) (CA INDEX NAME)



IT 214261-89-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of di-, tri-, and tetranuclear cyclobutenylidene chromium iron
complexes)
RN 214261-89-9 HCAPLUS
CN Chromium, pentacarbonyl[carbonyl(.eta.5-2,4-cyclopentadien-1-
yl)(triphenylphosphine)iron][.mu.3-[(4,4-dimethyl-1-cyclobutene-1,2-diyl-3-
ylidene)-1,2-ethynediyl]] [iodobis(triethylphosphine)platinum]-,
stereoisomer (9CI) (CA INDEX NAME)



L72 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1996:733807 HCAPLUS

DN 126:75049

TI 1,3-Heterobinuclear cyclobutenylidene complexes with an exocyclic C:C bond. Synthesis, structure, and spectroscopic properties

AU Fischer, Helmut; Leroux, Frederic; Stumpf, Ruediger; Roth, Gerhard

CS Fakultät Chemie, Universitaet Konstanz, Konstanz, D-78434, Germany

SO Chemische Berichte (1996), 129(12), 1475-1482

CODEN: CHBEAM; ISSN: 0009-2940

PB VCH

DT Journal

LA English

OS CASREACT 126:75049

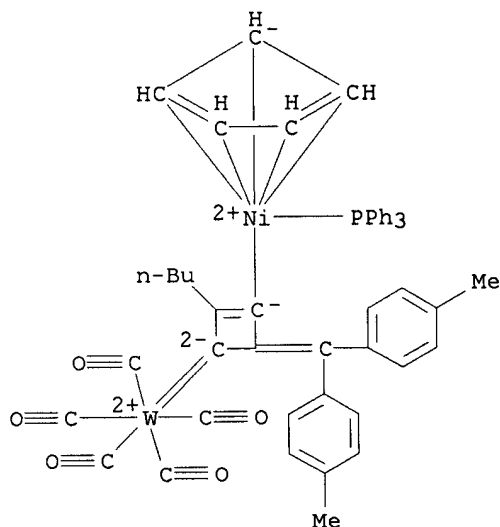
AB [(OC)5M:C:C(C6H4-4-R)2] (M = Cr, W; R = Me, MeO) reacts with [Cp(CO)2FeC.tplbond.CR1] (R1 = Bu, Ph), [Cp*(CO)2FeC.tplbond.CBu], [Cp(CO){P(OMe)3}FeC.tplbond.CBu], or [Cp(PPh3)NiC.tplbond.CBu] by cycloaddn. of the C.tplbond.C bond of the alkynyl complexes to the C.alpha.:C.beta. bond of the allenylidene ligand to give the cyclobutenylidene complexes I [M = Cr, W; R = Me, MeO; same R1; Y = FeCp(CO)2, FeCp[P(OMe)3](CO), NiCpPPh3] and II [M = Cr, R = Me; R1 = Bu; Y = FeCp*(CO)2]. The cycloaddn. is highly selective. The spectroscopic data of these 1,3-heterobinuclear complexes indicate a delocalized .pi.-system. X-ray structural anal. of I [M = Cr, R = Me, Y = FeCp(CO)2, FeCp[P(OMe)3](CO) and M = W, R = Me, Y = NiCpPPh3] reveals a butterfly conformation of the 4-membered ring with puckering angles of 142.degree., 152.degree., and 151.degree., resp. All complexes exhibit a moderate to strong neg. solvatochromic behavior. The extent of the solvatochromic effect depends on [(CO)5M] and Y and considerably decreases when C:C(C6H4-4-R)2 is replaced by, e.g., CMe2.

IT 185462-38-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; prepn. and solvatochromism of heterobinuclear cyclobutenylidene complexes)

RN 185462-38-8 HCAPLUS

CN Tungsten, [.mu.-[4-[bis(4-methylphenyl)methylene]-2-butyl-1-cyclobuten-1-yl-3-ylidene]]pentacarbonyl[(.eta.5-2,4-cyclopentadien-1-yl)(triphenylphosphine)nickel]- (9CI) (CA INDEX NAME)



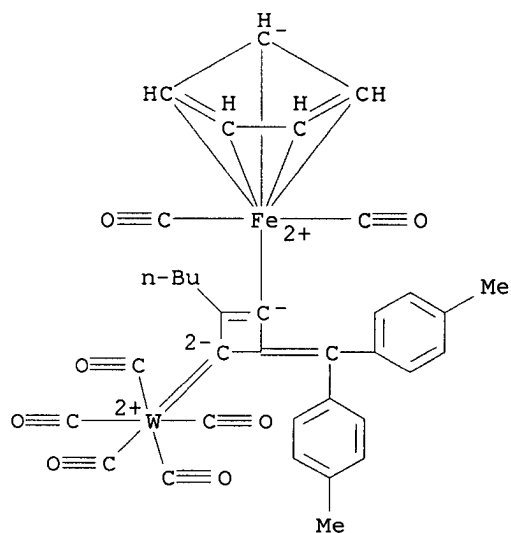
IT 185462-30-0P 185462-35-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and solvatochromism of heterobinuclear cyclobutenylidene complexes)

RN 185462-30-0 HCAPLUS

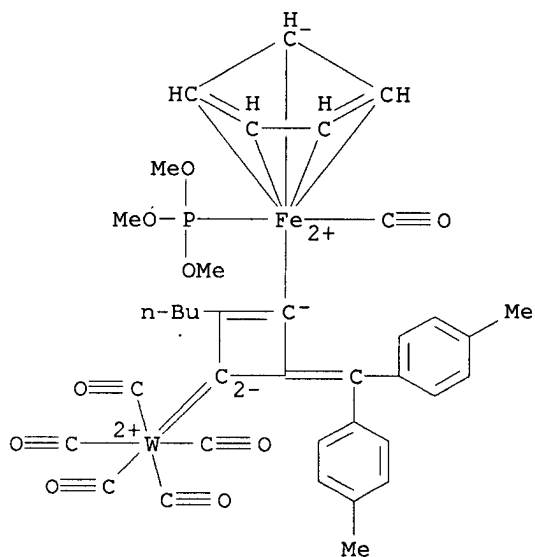
CN Tungsten, [.mu.-[4-[bis(4-methylphenyl)methylene]-2-butyl-1-cyclobuten-1-

yl-3-ylidene]]pentacarbonyl[dicarbonyl(.eta.5-2,4-cyclopentadien-1-yl)iron]- (9CI) (CA INDEX NAME)



RN 185462-35-5 HCAPLUS

CN Tungsten, [.mu.-[4-[bis(4-methylphenyl)methylene]-2-butyl-1-cyclobuten-1-yl-3-ylidene]]pentacarbonyl[carbonyl(.eta.5-2,4-cyclopentadien-1-yl)(trimethyl phosphite-.kappa.P)iron]- (9CI) (CA INDEX NAME)



L114 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2002 ACS

AN 1999:126456 HCAPLUS

DN 130:267546

TI A comprehensive study of [2 + 2] cycloadditions and ene reactions of alkynyl chromium and tungsten carbene complexes with enol ethers and ketene acetals and of the stereochemistry of the electrocyclic ring opening of cyclobutenyl carbene complexes

AU Wulff, William D.; Faron, Katherine L.; Su, Jing; Springer, James P.; Rheingold, Arnold L.

CS Searle Chemistry Laboratory, Department of Chemistry, University of Chicago, Chicago, IL, 60637, USA

SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (2), 197-219
CODEN: JCPRB4; ISSN: 0300-922X

PB Royal Society of Chemistry

DT Journal

LA English

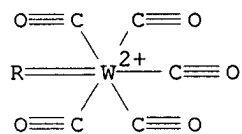
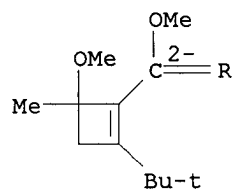
OS CASREACT 130:267546

AB The reactions of several alkynyl carbene complexes

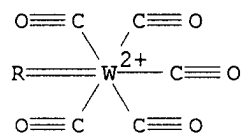
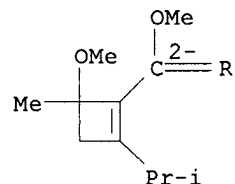
[(CO)5M:C(OMe)C.tplbond.CR1, M = Cr, W, R1 = Me, Me3Si, Ph, i-Pr, t-Bu] with a variety of acyclic enol ethers and ketene acetals [CH2:C(OR2)R3, R2 = Et, Me, i-Bu, SiMe2t-Bu, R3 = H, Me, EtO, p-MeC, 6H4] are examd. These reactions occur to give [2+2] cycloaddn. products in all cases except with R1 = Me3Si where ene products predominate. The cyclobutenyl carbene complexes produced in the [2+2] cycloaddns. undergo rapid electrocyclic ring-opening at room temp. when R3 = H to give butadienyl carbene complexes as the isolated products. The reactions of the alkynyl carbene complexes with cyclic enol ethers derived from cyclohexanone and cyclopentanone are more prone to give ene products than the acyclic enol ethers. Greater proportions of ene products are seen for six-membered than five-membered ring enol ethers and for silyl rather than alkyl enol ethers and for silyl rather than carbon substituents at R1. Only small differences are seen between chromium and tungsten complexes. The [2+2] cycloaddns. with the E- and Z-isomers of Et prop-1-enyl ether are stereo-specific with complexes in which R1 = Me but not with those with R1 = SiMe3. The cyclobutenyl carbene complexes from the latter reactions with tungsten derivs. were found to undergo stereoselective electrocyclic ring-opening at 70.degree. to give only Z,E-butadienyl carbene complexes which result from the conrotatory ring-opening in which the ethoxy group **rotates** in an outward direction. An E,E-isomer was also isolated from the thermolysis mixt.; however, it was shown not to be a primary product but rather the result of an isomerization of the Z,E-butadienyl carbene complex under the reaction conditions. The stereoselectivity of the electrocyclic ring-opening of these cyclobutenyl carbene complexes was the same as that found for their corresponding cyclobutenyl esters. In one case, an interesting cine-rearrangement of a cyclobutenyl carbene complex was obsd. The metal can be oxidatively removed from the cyclobutenyl carbene complexes to give the corresponding cyclobut-1-enyl esters in good yield. Thus, alkynyl carbene complexes can serve as synthons for alkynyl esters in [2+2] cycloaddns. with enol ethers and have the attractive feature of greatly increased reaction rates. Addnl. synthetic interest can be assocd. with processes in which the [2+2] cycloaddn. of the alkynyl carbene complex is coupled in tandem with other reactions of the carbene complex functionality in the cycloadducts. This is illustrated with Diels-Alder reactions of the butadienyl carbene complexes and cyclohexadienone annulations of a cyclobutenyl carbene complex.

RN 117799-96-9 HCAPLUS

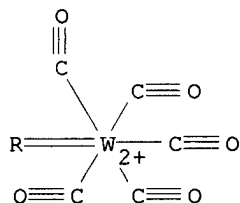
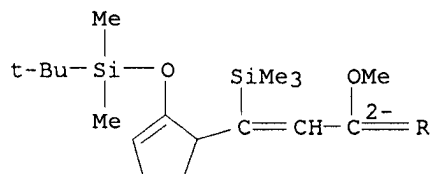
CN Tungsten, pentacarbonyl[[2-(1,1-dimethylethyl)-4-methoxy-4-methyl-1-cyclobuten-1-yl]methoxymethylene]-, (OC-6-21)- (9CI) (CA INDEX NAME)



RN 222173-20-8 HCAPLUS
 CN Tungsten, pentacarbonyl[methoxy[4-methoxy-4-methyl-2-(1-methylethyl)-1-cyclobuten-1-yl]methylene]-, (OC-6-21)- (9CI) (CA INDEX NAME)

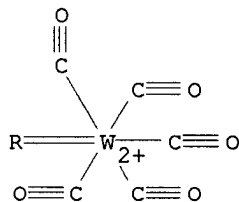
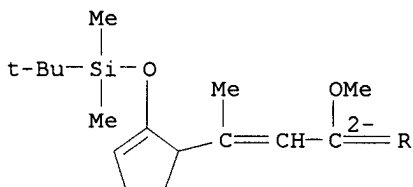


RN 128901-05-3 HCAPLUS
 CN Tungsten, pentacarbonyl[(2Z)-3-[2-[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-cyclopenten-1-yl]-1-methoxy-3-(trimethylsilyl)-2-propenylidene]-, (OC-6-21)- (9CI) (CA INDEX NAME)



RN 128901-07-5 HCAPLUS

CN Tungsten, pentacarbonyl{(2E)-3-[2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-cyclopenten-1-yl]-1-methoxy-2-butenylidene]-, (OC-6-21)-(9CI) (CA
INDEX NAME)



L119 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2002 ACS

AN 1983:438618 HCAPLUS

DN 99:38618

TI Metallocene complexes of cyclopentadienyl ylides

AU Holy, Norman L.; Nalesnik, Theodore; Warfield, Larry; Mojesky, Mark

CS Dep. Chem., Western Kentucky Univ., Bowling Green, KY, 42101, USA

SO J. Coord. Chem. (1983), 12(3), 157-62

CODEN: JCCMBQ; ISSN: 0095-8972

DT Journal

LA English

AB Several new transition metal complexes of the cyclopentadienyl ylides (CpPPh₃, CpSMe₂, CpPy; Cp = .eta.5-cyclopentadienyl; Py = pyridyl) are reported. Reactions of CpSMe₂ with MnCl₂, FeCl₂, CoCl₂ and NiX₂ (X = Cl, Br) leads to complexes in which the ylide:metal halide stoichiometry is 1:1. These complexes are assigned sandwich structures. Reaction of Pd(NO₃)₂ with CpSMe₂ yields a very air-sensitive compd. having a unique (CpSMe₂)₃Pd(NO₃)₂ stoichiometry. With HgX₂, CpSMe₂HgX₂ (X = Cl, Br, I) are formed; the Hg is bonded at C-3 of the cyclopentadienyl ring in the iodide deriv. Reaction of CpPPh₃ with FeCl₂ produces two derivs. which appear to have stoichiometries unique in iron metallocene chem.: (CpPPh₃)Fe₂Cl₄ and (CpPPh₃)Fe₂Cl₄.

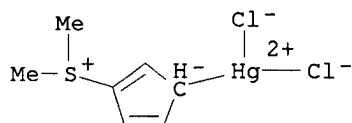
IT 86355-92-2P 86355-93-3P 86355-94-4P

86356-02-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

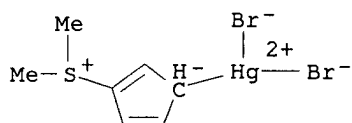
RN 86355-92-2 HCAPLUS

CN Mercury, dichloro[3-(dimethylsulfonio)-2,4-cyclopentadien-1-yl]- (9CI)
(CA INDEX NAME)



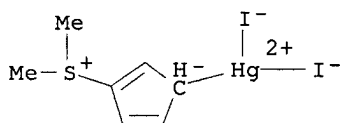
RN 86355-93-3 HCAPLUS

CN Mercury, dibromo[3-(dimethylsulfonio)-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)



RN 86355-94-4 HCAPLUS

CN Mercury, [3-(dimethylsulfonio)-2,4-cyclopentadien-1-yl]diiodo- (9CI) (CA INDEX NAME)



L119 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2002 ACS

AN 1981:462291 HCAPLUS

DN 95:62291

TI Halogenation, thallation, and mercuration of triphenylphosphonium and dimethylsulfonium cyclopentadienylides

AU Roberts, R. M. G.

CS Dep. Chem., Univ. Essex, Colchester, CO4 3SQ, Engl.

SO Tetrahedron (1980), 36(22), 3295-300

CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

AB Reaction of cyclopentadienylides I ($Z = \text{PPh}_3$, SMe_2) with $\text{CF}_3\text{CO}_2\text{H}$, AcOH , iodine, Br , Tl and Hg salts in both acidic and neutral media is reported. Addn. reactions predominated, with sterically controlled attack at C-2 in I ($Z = \text{SMe}_2$) and at C-3 in I ($Z = \text{PPh}_3$). Thallation and mercuration were studied in detail by NMR, and the reaction products were identified.

IT 77851-78-6P 77851-80-0P 77979-57-8P

77979-58-9P 77979-59-0P 77979-60-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

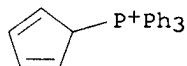
RN 77851-78-6 HCAPLUS

CN Phosphonium, 2,4-cyclopentadien-1-yltriphenyl-, potassium
(T-4)-tetrabromomercurate(2-) (1:1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 77851-77-5

CMF C23 H20 P



L119 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2002 ACS

AN 1981:462291 HCAPLUS

DN 95:62291

TI Halogenation, thallation, and mercuration of triphenylphosphonium and dimethylsulfonium cyclopentadienylides

AU Roberts, R. M. G.

CS Dep. Chem., Univ. Essex, Colchester, CO4 3SQ, Engl.

SO Tetrahedron (1980), 36(22), 3295-300

CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

AB Reaction of cyclopentadienylides I (Z = PPh₃, SMe₂) with CF₃CO₂H, AcOH, iodine, Br, Tl and Hg salts in both acidic and neutral media is reported. Addn. reactions predominated, with sterically controlled attack at C-2 in I (Z = SMe₂) and at C-3 in I (Z = PPh₃). Thallation and mercuration were studied in detail by NMR, and the reaction products were identified.

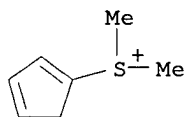
RN 77851-80-0 HCAPLUS

CN Sulfonium, 1,3-cyclopentadien-1-yl dimethyl-, tribromomercurate(1-) (9CI)
(CA INDEX NAME)

CM 1

CRN 77851-79-7

CMF C7 H11 S

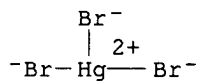


CM 2

CRN 21388-05-6

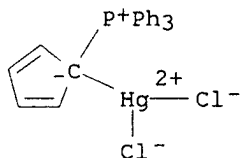
CMF Br₃ Hg

CCI CCS



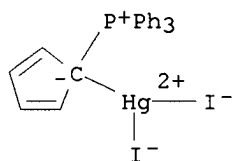
RN 77979-58-9 HCAPLUS

CN Mercury, dichloro[triphenylphosphonium (1-.eta.)-2,4-cyclopentadien-1-ylide]- (9CI) (CA INDEX NAME)



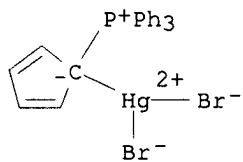
RN 77979-59-0 HCAPLUS

CN Mercury, diiodo[triphenylphosphonium (1-.eta.)-2,4-cyclopentadien-1-ylide]- (9CI) (CA INDEX NAME)



RN 77979-60-3 HCAPLUS

CN Mercury, dibromo[triphenylphosphonium (1-eta.)-2,4-cyclopentadien-1-ylide]- (9CI) (CA INDEX NAME)



L123 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2002 ACS

AN 1995:732403 HCAPLUS

DN 123:126027

TI The microwave spectrum of **cyclopentadienyl** vanadium tetracarbonyl, a fluxional molecule

AU McKay, R. T.; Hubbard, J. L.; Kukolich, S. G.

CS Dep. Chem., Univ. Arizona, Tucson, AZ, 85721, USA

SO J. Mol. Spectrosc. (1995), 172(2), 378-83

CODEN: JMOSA3; ISSN: 0022-2852

DT Journal

LA English

AB The microwave spectrum of the sym.-top, **transition metal** complex $n^5\text{-C}_5\text{H}_5\text{V}(\text{CO})_4$ was measured in the 3-11 GHz range using a Flygare-Balle-type spectrometer. The mol. parameters obtained from the spectra are $B = 640.429(5)$ MHz, $eqQ(51\text{V}) = -4.77(6)$ MHz, and $DJ = 0.17(4)$ kHz. Approx. one-half of the measured transition frequencies did not fit the pattern expected for a sym.-top, rigid **rotor** with quadrupole coupling and are believed to be due to the effects of a low-frequency vibrational mode. In addn., the line centers for the rotational transitions which were fit to the sym.-top model showed systematic deviations of approx. ± 0.20 kHz. It is proposed that these two anomalies are due to low-frequency CO bending modes which result in deviations from the C_{4v} symmetry of the $\text{V}(\text{CO})_4$ group.

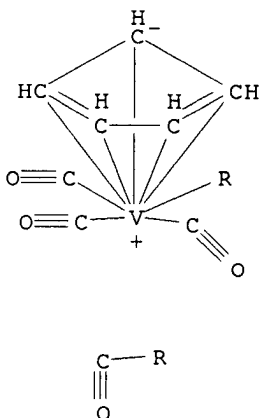
IT 12108-04-2, **Cyclopentadienyl** vanadium tetracarbonyl

RL: PRP (Properties)

(microwave spectrum of **cyclopentadienyl** vanadium tetracarbonyl)

RN 12108-04-2 HCAPLUS

CN Vanadium, tetracarbonyl(.eta.5-2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



IT 7440-62-2, Vanadium-51, properties

RL: PRP (Properties)

(quadrupole coupling; microwave spectrum of **cyclopentadienyl** vanadium tetracarbonyl)

RN 7440-62-2 HCAPLUS

CN Vanadium (8CI, 9CI) (CA INDEX NAME)

V

L123 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2002 ACS

AN 1978:6224 HCAPLUS

DN 88:6224

TI Conformational preferences and rotational barriers in polyene-ML3
transition metal complexes

AU Albright, Thomas A.; Hofmann, Peter; Hoffmann, Roald

CS Dep. Chem., Cornell Univ., Ithaca, N. Y., USA

SO J. Am. Chem. Soc. (1977), 99(23), 7546-57

CODEN: JACSAT

DT Journal

LA English

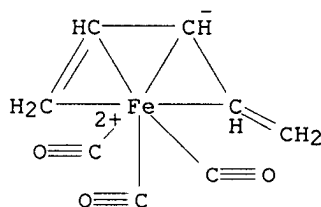
AB Conformational preferences, the magnitudes of rotational barriers, and their phys. origin are analyzed for a series of cyclic and acyclic polyene-ML3 *****transition*** metal** complexes. Described in detail are the barriers in trimethylenemethane, benzene, and pentadienyl-M(CO)₃ compds. The treatment is then extended to other polyene systems and comparisons are made with available exptl. information. The barriers in these mols. span a range from large (.gtoreq.20 kcal/mol) in octahedral mols. and trimethylenemethane complexes, through intermediate values (5-15 kcal/mol) in butadiene, pentadienyl, and hexatriene-M(CO)₃, to tiny barriers in **cyclopentadienyl** and benzene complexes. These barriers were analyzed via a reconstitution of the orbitals of the mol. from the valence orbitals of the polyene and ML3 fragments. The symmetry of the fragment **rotors** plays a crucial role in setting the size of the barrier. However, the substantial threefold barrier component is set not so much by interligand repulsions as by intrinsic overlap difference between the fragment orbitals in the various conformations. The same controlling factor differentiates between octahedral and trigonal prismatic Cr(CO)₆; the more a polyene-M(CO)₃ complex resembles an octahedron the greater will be the barrier to internal rotation in that mol. A benzenechromium tricarbonyl model shows how perturbations within the .pi. framework dictate the magnitude of the barrier and conformational preferences. Substantial barriers may be expected when the substitution pattern reinforces local octahedral symmetry. Variations within the ML3 framework by changing the ligand from a .pi. acceptor to a .pi. donor and altering the L-M-L angle are also described.

IT 65209-16-7 65209-17-8

RL: PRP (Properties)

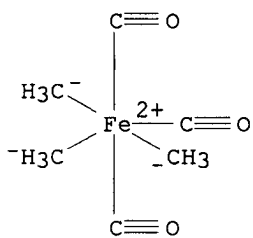
(rotational barrier of, calcn. of)

RN 65209-16-7 HCAPLUS

CN Iron(1+), tricarbonyl[(1,2-.eta.)-1-(.eta.2-ethenyl)-2-propenyl]- (9CI)
(CA INDEX NAME)

RN 65209-17-8 HCAPLUS

CN Ferrate(1-), tricarbonyltrimethyl- (9CI) (CA INDEX NAME)



L72 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 2000:757322 HCAPLUS

DN 134:71679

TI Organic syntheses via transition metal complexes. CV. Regiocontrol of annelation of cyclopentene-1-thiones and cyclopenten-1-ones to alkenes with the aid of (1-alkynyl)carbene complexes (M = Cr, W)

AU Wu, He-Ping; Aumann, Rudolf; Venne-Dunker, Sabine; Saarenketo, Pauli
CS Organisch-Chemisches Institut der Universitat Munster, Munster, 48149, Germany

SO European Journal of Organic Chemistry (2000), (20), 3463-3473

CODEN: EJOCFK; ISSN: 1434-193X

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

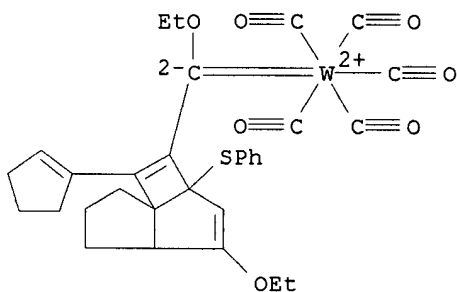
AB Bicyclic olefins contg. a 1-oxy-3-thiocyclopentadiene unit were obtained with high regioselectivity from [2-(cycloalk-1-enyl)-1-alkynyl]carbene complexes I (M = W, X = CH₂, CH₂CH₂, CH₂CH₂CH₂; M = Cr, X = CH₂CH₂) and thiols under mild conditions. If the reaction was performed in a protic solvent like ethanol, the produced allylthiocyclopentadienes spontaneously underwent a thio Claisen rearrangement to give cyclopentene-1-thione complexes in 62-72% yields. In nonprotic solvents, addnl. cyclopentene-1-thione complexes were obtained as a result of the incorporation of two and three allylthiol units, resp. Arylthiotetrahydroindene complexes could be isolated in 76-79% yields. The corresponding tetrahydropentalene deriv. was unstable, but could be trapped by [2+2] cycloaddn. of (1-alkynyl)carbene complex to give a stable (cyclobutenyl)carbene complex. Hydrolysis of arylthiotetrahydroindene complexes afforded cyclopenten-1-ones. The crystal structures of (7a-allyl-3-ethoxy-3a,4,5,6,7,7a-hexahydroindene-1-thione-S)pentacarbonyltungsten, (1S*,4R*,7R*)-2-(cyclopent-1-enyl)-6-ethoxy-3-(1,1,1,1,1-pentacarbonyl-2-ethoxy-1-tungsta-2-ethenyl)-4-phenylthiospirotricyclo[5.3.0.1,4.0.1,7]deca-2,5-diene, and pentacarbonyl(1-ethoxy-3-phenylthio-2,4,5,6-tetrahydropentalene-S)tungsten were detd.

IT 314069-92-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of)

RN 314069-92-6 HCAPLUS

CN Tungsten, pentacarbonyl[[rel-(2aR,4aR,7aS)-1-(1-cyclopenten-1-yl)-4-ethoxy-2a,4a,6,7-tetrahydro-2a-(phenylthio)-5H-cyclobuta[c]pentalen-2-yl]ethoxymethylene]-, (OC-6-21)- (9CI) (CA INDEX NAME)



L72 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 2000:243706 HCAPLUS

DN 132:347687

TI Organic syntheses via transition metal complexes, CII.

1,3-Dioxycyclopentadienes from (1-alkynyl)carbene tungsten complexes - domino cyclization/cycloaddition reactions

AU Wu, He-Ping; Aumann, Rudolf; Frohlich, Roland; Wibbeling, Birgit

CS Organisch-Chemisches Institut der Universitat Munster, Munster, D-48149, Germany

SO European Journal of Organic Chemistry (2000), (7), 1183-1192

CODEN: EJOCFK; ISSN: 1434-193X

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

OS CASREACT 132:347687

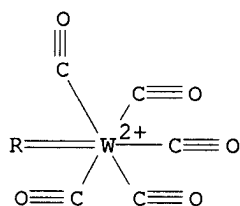
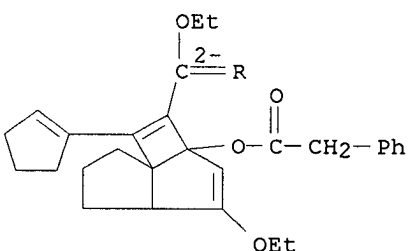
AB 1,3-Dioxytetrahydropentalenes (9) were generated by base-catalyzed addn. of protic O nucleophiles ROH 6a-g (RO = carboxy or phenyloxy) to the [2-(1-cyclopentenyl)ethynyl]carbene W complex 3. Compds. 9 are highly reactive and afford (cyclobutenyl)carbene complexes 12a-g through spontaneous [2+2] cycloaddn. to a 2nd mol. of the (1-alkynyl)carbene complex 3. Thermolysis of compds. 12 generates indeno[b]-spirotricyclo[5.3.0.0]decadienes 18 through .pi.-cyclization of the 1-tungsta-1,3,5-hexatriene unit involving insertion of CO into the W:C bond. The crystal and mol. structures of 12b (shown as I; R = PhCH₂C(O)), 18f (shown as II; R = Ph) and [Et₃NH][(OC)₅W(O₂CC₆H₄tBu-4)] were detd. by x-ray crystallog.

IT 269404-47-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and crystal structure of)

RN 269404-47-9 HCAPLUS

CN Tungsten, pentacarbonyl[[rel-(2aR,4aR,7aS)-1-(1-cyclopenten-1-yl)-4-ethoxy-2a,4a,6,7-tetrahydro-2a-[(phenylacetyl)oxy]-5H-cyclobuta[c]pentalen-2-yl]ethoxymethylene]-, (OC-6-21)- (9CI) (CA INDEX NAME)

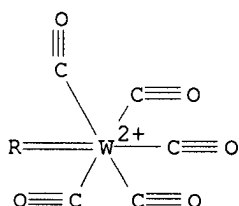
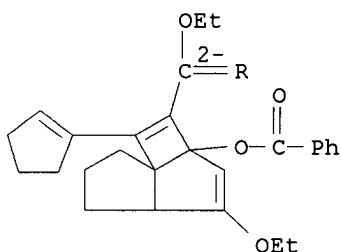


IT 269404-48-0P 269404-50-4P

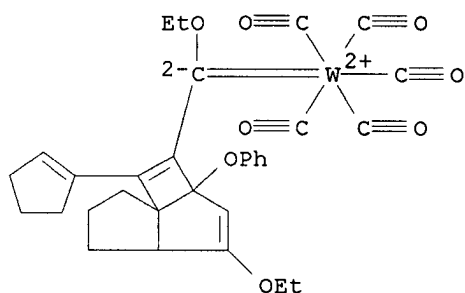
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and thermal cyclization/demetallation/carbon monoxide insertion of)

RN 269404-48-0 HCAPLUS

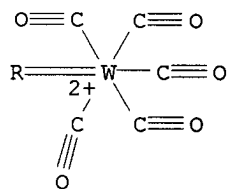
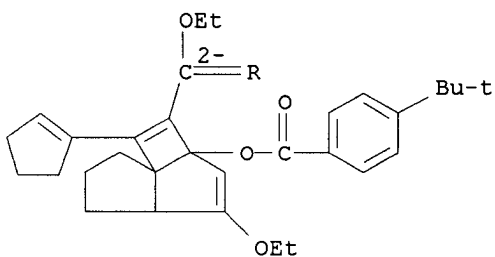
CN Tungsten, [[rel-(2aR,4aR,7aS)-2a-(benzoyloxy)-1-(1-cyclopenten-1-yl)-4-ethoxy-2a,4a,6,7-tetrahydro-5H-cyclobuta[c]pentalen-2-yl]ethoxymethylene]pentacarbonyl-, (OC-6-21)- (9CI) (CA INDEX NAME)



RN 269404-50-4 HCAPLUS
 CN Tungsten, pentacarbonyl[[rel-(2aR,4aR,7aS)-1-(1-cyclopenten-1-yl)-4-ethoxy-2a,4a,6,7-tetrahydro-2a-phenoxycyclobuta[c]pentalen-2-yl]ethoxymethylene]-, (OC-6-21)- (9CI) (CA INDEX NAME)

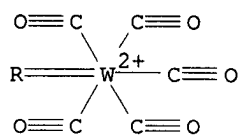
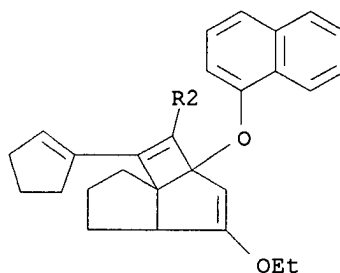


IT **269404-49-1P 269404-51-5P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 269404-49-1 HCAPLUS
 CN Tungsten, pentacarbonyl[[rel-(2aR,4aR,7aS)-1-(1-cyclopenten-1-yl)-2a-[[4-(1,1-dimethylethyl)benzoyl]oxy]-4-ethoxy-2a,4a,6,7-tetrahydro-5H-cyclobuta[c]pentalen-2-yl]ethoxymethylene]-, (OC-6-21)- (9CI) (CA INDEX NAME)

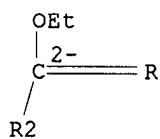


RN 269404-51-5 HCAPLUS
 CN Tungsten, pentacarbonyl[[rel-(2aR,4aR,7aS)-1-(1-cyclopenten-1-yl)-4-ethoxy-2a,4a,6,7-tetrahydro-2a-(1-naphthalenyloxy)-5H-cyclobuta[c]pentalen-2-yl]ethoxymethylene]-, (OC-6-21)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

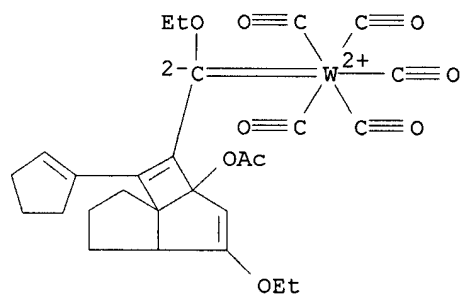


IT 269404-46-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(prepn., thermal cyclization/demetalation/carbon monoxide insertion and
oxidative demetalation using DMSO)

RN 269404-46-8 HCAPLUS

CN Tungsten, [[rel-(2aR,4aR,7aS)-2a-(acetyloxy)-1-(1-cyclopenten-1-yl)-4-
ethoxy-2a,4a,6,7-tetrahydro-5H-cyclobuta[c]pentalen-2-
yl]ethoxymethylene]pentacarbonyl-, (OC-6-21)- (9CI) (CA INDEX NAME)

L2 ANSWER 1 OF 1 HCAOLD COPYRIGHT 2002 ACS
 AN CA54:24457b CAOLD
 TI reaction of cyclopropane hydrocarbons with mercuric salts - (XI) opening
 of the three-membered ring in bicyclo[0.1.n]alkanes (n=2,3 and 4)
 AU Levina, R. Ya.; Kostin, V. N.; Ustynyuk, T. K.
 IT 92-51-3 185-94-4 286-08-8 98070-73-6 98336-55-1 98434-63-0
 98434-77-6 98485-73-5 98880-64-9 99419-49-5 127544-81-4

Chemical
 Abstracts

1960

24457

10D—Alicyclic

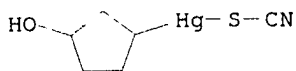
acid. The cis-joining of the lactone and cyclohexyl rings indicated the β -configuration of the epoxy group in VII. The bromohydroxy acid derived from VII had 2-HO group in cis position relative to the aceturic acid residue, since treatment with 10% HBr-AcOH gave bromolactone III. α X, m. 192-3°, formed the acetate, m. 129-30°.

G. M. Kosolapoff

Reaction of cyclopropane hydrocarbons with mercuric salts. XI. Opening of the three-membered ring in bicyclo[0.1.n]alkanes ($n = 2, 3$, and 4). R. Ya. Levina, V. N. Kostin, and T. K. Ustynyuk (State Univ., Moscow). *Zhur. Obshchei Khim.* 30, 359-63(1960); cf. *CA* 54, 9791h.—Opening of the 3-membered ring by $\text{Hg}(\text{OAc})_2$ occurred in bicyclic systems with a 3-membered ring and the reaction was used to identify such systems. Reaction of 4 g. bicyclo[0.1.2]pentane with 22.67 g. $\text{Hg}(\text{OAc})_2$ in 100 ml. H_2O at 0° gave 82% 3-hydroxycyclopentylmercuric acetate, an oil; with KCl this gave the chloride, m. 97-8°; KBr gave the bromide, m. 129-30°; thiocyanate m. 110-11°. Heating the acetate with Zn dust gave some Hg and 85% cyclopentanone. Similarly, bicyclo[0.1.3]hexane and $\text{Hg}(\text{OAc})_2$ (few hrs. at room temp.) gave 60% 2-hydroxycyclopentylmethylmercuric bromide, m. 151-2° (after treatment of the mixt. with KBr). Bicyclo[0.1.4]heptane gave 86% 2-hydroxycyclohexylmethylmercuric acetate, m. 129-30°; chloride m. 122-3°; bromide m. 114-15°. Heating the acetate with Zn dust gave 2-methylcyclohexanone. The other products of the above reactions with Zn were the corresponding alcs., which were identified conventionally.

G. M. Kosolapoff

L61 ANSWER 1 OF 19 REGISTRY COPYRIGHT 2002 ACS
 RN 127544-81-4 REGISTRY
 CN Cyclopentanol, 3-thiocyanatomercuri- (6CI) (CA INDEX NAME)
 MF C6 H9 Hg N O S
 SR CAOLD
 LC STN Files: CAOLD



example
 of
 Alg - 3

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

08/01/2002

Serial No.:09/812,647

FILE 'REGISTRY' ENTERED AT 09:07:12 ON 01 AUG 2002
L1 STRUCTURE UPLOADED
L2 0 S L1 SSS SAM
L3 27 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 09:12:06 ON 01 AUG 2002
L4 0 S L2
L5 11 S L3

FILE 'MARPAT' ENTERED AT 09:13:47 ON 01 AUG 2002
L6 124 S L1 SSS FULL

08/01/2002

Serial No.:09/812,647

=> D L1

L1 HAS NO ANSWERS

L1 STR



M

L5 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2002 ACS

AN 2002:421732 HCAPLUS

DN 136:386261

TI Ansa-zirconocenes functionalized on their cyclosilane bridges, their preparation and activity as polymerization catalysts

IN Lemenovskii, D. A.; Krut'ko, D. P.; Borzov, M. V.; Brusova, G. P.; Veksler, E. N.; Nedorezova, P. M.; Tsvetkova, V. I.

PA Institut Khimicheskoi Fiziki RAN im. N. N. Semenova, Russia

SO Russ., No pp. given

CODEN: RUXXE7

DT Patent

LA Russian

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	RU 2160277	C1	20001210	RU 1999-113532	19990621

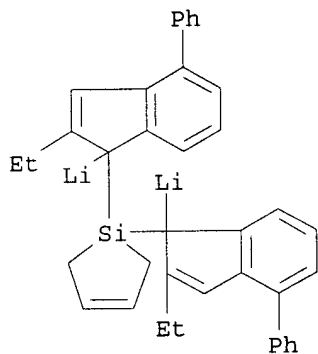
OS CASREACT 136:386261; MARPAT 136:386261

AB Ansa-zirconocenes functionalized on their cyclosilane bridges I [R1 = H, Me, Et; R2 = H, (un)branched C1-4 alkyl, aryl; A = BC8H14, MR3; M = Sn, Si; R = (un)branched C1-4 alkyl, aryl], useful as catalysts for prepn. of polyolefins, are claimed. Also claimed is a method for prepn. of I comprising synthesizing substituted indene, prepg. the Li salt of the indene and reaction of the latter with 1,1-dichloro-2,5-dihydrosilole in Et2O and subsequently treating the resulting dilithium salt of the corresponding Si-bridged bis-indenyl ligand with ZrCl4 to give the corresponding zirconocene and heating it in THF with an alkyl(aryl)deriv. of B monohydride, Sn or Si. This method makes it possible to obtain high yields of intermediates and desired products and permits increasing content of active racemic form in metallic complex. The resulting compds. have high catalytic activity and stereoselectivity in the polymn. of propylene. In an example, reaction of indenyllithium with 1,1-dichloro-2,5-dihydrosilole gave the bis(indenyl)silole bidentate ligand which formed a dilithium salt-Et2O adduct upon treatment with BuLi in Et2O, and complexation of the latter with ZrCl4 in PhMe and subsequent functionalization with 9-BBN in THF gave I (R1 = R2 = H, AH = 9-BBN), and its catalytic activity for polymn. of propylene was demonstrated.

IT **426820-10-2P 426820-11-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and complexation with zirconium tetrachloride)

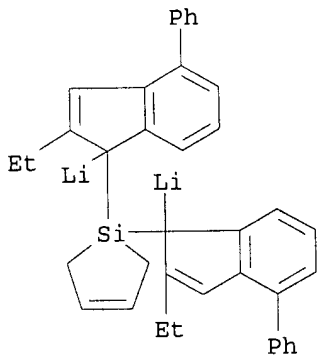
RN 426820-10-2 HCAPLUS

CN Lithium, [μ -(silacyclopent-3-en-1-ylidenebis(2-ethyl-4-phenyl-1H-inden-1-ylidene))]di- (9CI) (CA INDEX NAME)

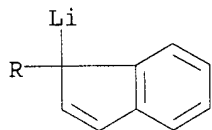
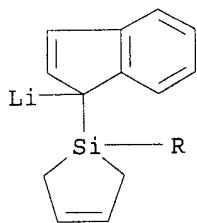


08/01/2002

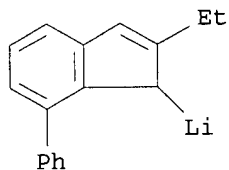
Serial No.:09/812,647



RN 426820-11-3 HCAPLUS
CN Lithium, [μ -(silacyclopent-3-en-1-ylidenedi-1H-inden-1-ylidene)]di-
(9CI) (CA INDEX NAME)



IT 426820-06-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and silylation of, with 1,1-dichloro-2,5-dihydrosilole)
RN 426820-06-6 HCAPLUS
CN Lithium, (2-ethyl-7-phenyl-1H-inden-1-yl)- (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2002 ACS
AN 2002:416502 HCAPLUS
DN 136:386260
TI Ansa-zirconocenes with an unsaturated cyclosilane bridge, their

08/01/2002

Serial No.:09/812,647

preparation and activity as polymerization catalysts

IN Lemenovskii, D. A.; Avtomonov, E. V.; Krut'ko, D. P.; Borzov, M. V.; Kazennova, N. B.; Tsvetkova, V. I.; Nedorezova, P. M.; Aladyshev, A. M.; Savinov, D. V.

PA Institut Khimicheskoi Fiziki im. N. N. Semenova RAN, Russia

SO Russ., No pp. given
CODEN: RUXXE7

DT Patent

LA Russian

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	RU 2160276	C1	20001210	RU 1999-113531	19990621

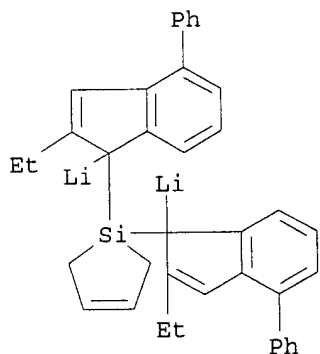
OS CASREACT 136:386260; MARPAT 136:386260

AB Ansa-zirconocenes having an unsatd. cyclosilane bridge I (R1 = H, Me, Et; R2 = H, (un)branched C1-4 alkyl, aryl), useful as polymn. catalysts for polyolefin prepn., are claimed. Also claimed is a method for prepn. of I by reaction of a lithium deriv. of indene with 1,1-dichloro-2,5-dihydrosilole in Et2O to give a bis-indenyl ligand having a cyclosilane bridge; subsequent dilithiation of the bis-indenyl ligand thus obtained affords a salt which exists as a cryst. adduct of Et2O, which upon treatment with ZrCl4 affords the desired product with high yield. Compds. I have high catalytic activity and stereoselectivity in polymn. reactions as mixts. of rac (active) and meso (inactive) forms. In an example, lithiation of 2-ethyl-4-phenylindene (prepn. given) with BuLi and subsequent silylation with 1,1-dichloro-2,5-dihydrosilole gave nearly quant. the bidentate ligand 1,1-bis(2-ethyl-4-phenyl-1-yl)-2,5-dihydrosilole which formed 70% of a cryst. salt-Et2O adduct upon dilithiation; treating the latter with ZrCl4 in PhMe gave 67% I (R1 = Et, R2 = Ph) as a 2:1 mixt. of rac and meso isomers, and these demonstrated improved catalytic activity in the polymn. of propylene over known zirconocene catalysts.

IT **426820-10-2P 426820-11-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and complexation of, with zirconium tetrachloride)

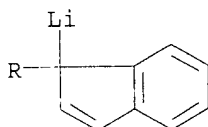
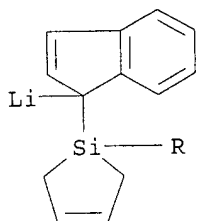
RN 426820-10-2 HCAPLUS

CN Lithium, [μ -(silacyclopent-3-en-1-ylidenebis(2-ethyl-4-phenyl-1H-inden-1-ylidene))]di- (9CI) (CA INDEX NAME)



RN 426820-11-3 HCAPLUS

CN Lithium, [μ -(silacyclopent-3-en-1-ylidenedi-1H-inden-1-ylidene))]di- (9CI) (CA INDEX NAME)



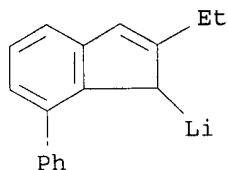
IT **426820-06-6P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and silylation of, with 1,1-dichloro-2,5-dihydrosilole)

RN 426820-06-6 HCAPLUS

CN Lithium, (2-ethyl-7-phenyl-1H-inden-1-yl)- (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2002 ACS

AN 2002:250235 HCAPLUS

DN 137:6252

TI Synthesis, Characterization, and Thermochemistry of (.eta.1-C13H9)Mn(CO)5 and (.eta.5-C13H9)Mn(CO)3

AU Decken, Andreas; MacKay, Andrew J.; Brown, Martin J.; Bottomley, Frank

CS Department of Chemistry, University of New Brunswick, Fredericton, NB, E3B 6E2, Can.

SO Organometallics (2002), 21(9), 2006-2009

CODEN: ORGND7; ISSN: 0276-7333

PB American Chemical Society

DT Journal

LA English

AB Reaction of LiC13H9 with Mn(CO)5Br at -78.degree. gave (.eta.1-C13H9)Mn(CO)5, 2. Thermal rearrangement of 2 yielded (.eta.5-C13H9)Mn(CO)3, 1, 9,9'-bifluorene, 3, and Mn2(CO)10, 4. The product distribution was controlled by the electron donor capacity of the reaction medium. The crystal structures of 1 and 2 were detd.

IT **433264-35-8P**

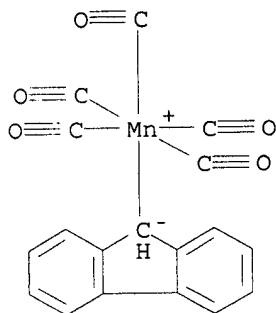
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn., crystal structure and thermal rearrangement of)

08/01/2002

Serial No.:09/812,647

RN 433264-35-8 HCAPLUS
 CN Manganese, pentacarbonyl-9H-fluoren-9-yl-, (OC-6-21)- (9CI) (CA INDEX NAME)



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2002 ACS

AN 2002:233098 HCAPLUS

DN 136:279567

TI Method for preparation of high-purity metallocene compounds using new organometallic complexes as intermediates

IN Kogure, Takeshi; Hori, Junichi

PA Kanto Chemical Co., Inc, Japan

SO Jpn. Kokai Tokkyo Koho, 15 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2002088092	A2	20020327	JP 2000-276187	20000912
OS	CASREACT 136:279567; MARPAT 136:279567				
AB	<p>An industrial process for high-purity metallocene compds. in good yields is provided, which solves the problem of low yields resulting from the use of a large quantity of org. solvent for extg. metal complexes and decompn. caused by washing with alc. solvent in synthesis of metallocene compds. sparingly sol. in org. solvent. The metallocene compds. [I; M = group 4 transition metal optionally coordinated to 1-2 of ether or amine ligand(s); X = halo; R1 - R10 = H, C1-30 alkyl, aryl; provided that at least one of the combination of R1 and R2, R2 and R3, R3 and R4, R5 and R6, R6 and R7, R7 and R8, and R9 and R10 is linked to each other to form an arom. ring] are prepd. by reaction of bisindene alkali or alk. earth metal salt (II; R1 - R10 = same as above; B = alkali or alk. earth metal cation) with transition metal compds. represented by formula [(R12)nR11A]2MX2 (A = atoms independently selected from group 15 and 16 atoms; n is 0, when A is the group 15 atom; n is 1 when A is the group 16 atom; R11 = C1-10 hydrocarbon group optionally contg. halo, N, P, O, and S, aryl optionally contg. halo substituent; R12 = alkyl or aryl optionally possessing C1-10 hydrocarbon group optionally contg. halo, N, P, O, and S; or R11 and R12 are linked to each other to form a ring contg. A or A and M; M, X = same as above) and halogenation of the resulting intermediate metallocene compds. (III; R1 - R12, M, n = same as above). This process uses the above transition metal metallocene compds. III as intermediates which are readily sol. in org. solvent, and enable inorg. salts to be</p>				

removed at this reaction stage giving the intermediates prior to halogenation, and the subsequent halogenation of III efficiently gives high-purity metallocene compds. free from inorg. salts. These metallocene compds. I are useful as catalysts for org. synthesis. Thus, 0.50 g isopropylidene(1-indene)[1-(4,5-benzoindene)] and 10 mL THF were added to a 100 mL Schlenk flask, cooled at 0.degree., treated with 2.01 mL 1.59 M BuLi/hexane, and stirred for 4 h to give a reaction soln. contg. isopropylidene(1-indene)[1-(4,5-benzoindene)] dilithium salt which was added to 0.82 g bis(N-methylanilido)zirconium dichloride bistetrahydrofuran complex in 20 mL Schlenk flask, stirred for 3 h, and concd. to give a sticky solid. To the solid was added 40 mL CH₂Cl₂ and insol. LiCl was removed by filtration and the mother liquor was concd. to give 80.0% isopropylidene(1-indene)[1-(4,5-benzoindene)]zirconium bis(N-methylanilide) as red powder which (0.78 g) was treated with 10 mL CH₂Cl₂ and 0.254 g dimethylamine hydrochloride and stirred for 1 h to give 60% isopropylidene(1-indene)[1-(4,5-benzoindene)]zirconium dichloride.

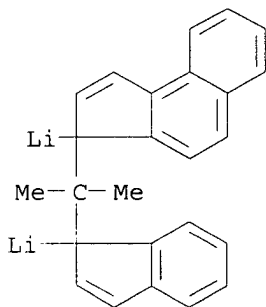
IT 405508-37-4P, Isopropylidene(1-indene)[1-(4,5-benzoindene)] dilithium salt 405508-39-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(method for prepn. of high-purity metallocene compds. as catalysts for org. synthesis using new organometallic complexes as intermediates)

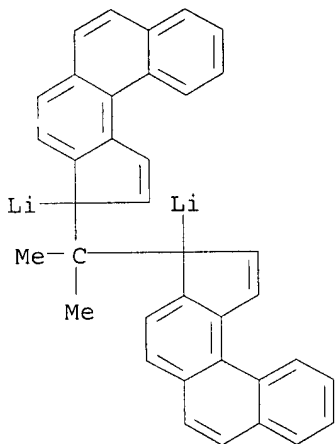
RN 405508-37-4 HCAPLUS

CN Lithium, [.mu.-[3H-benz[e]inden-3-ylidene(1-methylethylidene)-1H-inden-1-ylidene]]di- (9CI) (CA INDEX NAME)



RN 405508-39-6 HCAPLUS

CN Lithium, [.mu.-[(1-methylethylidene)bis(3H-cyclopenta[c]phenanthren-3-ylidene)]]di- (9CI) (CA INDEX NAME)

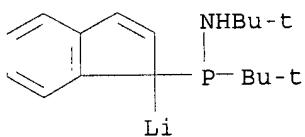


L5 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2002 ACS
 AN 2002:210180 HCAPLUS
 TI Alkyl(amino)- and alkyl(chloro)phosphino-substituted cyclopentadienyl
 complexes of titanium and zirconium
 AU Kotov, Vasily V.; Avtomonov, Evgeni V.; Sundermeyer, Jorg; Harms, Klaus;
 Lemenovskii, Dmitry A.
 CS Department of Chemistry, M. V. Lomonosov Moscow State University, Moscow,
 119899, Russia
 SO European Journal of Inorganic Chemistry (2002), (3), 678-691
 CODEN: EJICFO; ISSN: 1434-1948
 PB Wiley-VCH Verlag GmbH
 DT Journal
 LA English
 AB Phosphino-substituted cyclopentadienes of the type $[RnCp-PR(NR_1R_2/Cl)]$
 (1-22) ($R = \text{Alk}, \text{Ar}$; $R_1, R_2 = \text{H}, \text{Alk}, \text{Ar}, \text{SiR}_3$; $RnCp = \text{tBuCp}, \text{Me}_4\text{Cp}, \text{Ind},$
 $\text{Me}_6\text{Ind}, \text{Flu}$) can be synthesized by reaction of alkylchlorophosphines and
 alkyl(amino)chlorophosphines with alkali metal cyclopentadienides. The
 method used is a general one and provides high isolated yields of the
 target compds. The phosphinocyclopentadienes can easily be deprotonated
 by strong bases (e.g. $n\text{BuLi}$, PhCH_2K , Ph_2CHK) and the potassium salts
 $[RnCp-PR(NR_1R_2)]K$ (25-28) are efficiently transmetalated by Me_3SnCl . A
 subsequent reaction with $\text{TiCl}_4(L)_2$ and $\text{ZrCl}_4(L)_2$ ($L = \text{THF},$
 tetrahydrothiophene, Me_3P) affords new half-sandwich complexes
 $[\{\text{Me}_4\text{Cp-PtBu}(\text{NET}_2)\}\text{TiCl}_3]$ (36), $[\{\text{Me}_4\text{Cp-PtBu}(\text{NET}_2)\}\text{TiCl}_3]$ (37) and
 $[\{\text{tBuCp-PtBu}(\text{NET}_2)\}\text{TiCl}_3]$ (38) in moderate yields. The reaction of
 $[\text{tBuCp-PtBu}(\text{Cl})]$ (6) with TiCl_4 in the presence of Et_3N at low temp.
 yields the half-sandwich complex $[\{\text{tBuCp-PtBu}(\text{Cl})\}\text{TiCl}_3]$ (39) quant.;
 $[(\text{Cp-PtBuCl})_2\text{CMe}_2]$ (11) reacts similarly and gives, dependent on the
 reagent ratio, either the homobimetallic deriv. $[(\text{Cp-PtBuCl})_2\text{CMe}_2]\{\text{TiCl}_3\}_2$ (40) (1:2 ratio) or the ansa complex
 $[(\text{Cp-PtBuCl})_2\text{CMe}_2]\text{TiCl}_2$ (41) (1:1 ratio). The scope of this reaction
 could not be extended to sterically more demanding cyclopentadienyl
 derivs. Treatment of $[\{\text{tBuCp-PtBu}(\text{Cl})\}\text{TiCl}_3]$ (39) by $\text{LiN}(\text{H})\text{tBu}$ in the
 presence of Et_3N leads to the formation of the constrained geometry
 complex $[\{\text{tBuCp-PtBu}(\text{NtBu})\}\text{TiCl}_2]$ (42) in a high yield. All synthesized
 compds. were characterized by NMR spectroscopy, mass spectrometry and
 elemental analyses. The crystal structures of the ligand precursor
 $[\text{Me}_6\text{Ind-PtBu}(\text{NtBu})]$ (15) and that of $[\{\text{Me}_4\text{Cp-PtBu}(\text{NET}_2)\}\text{TiCl}_3]$ (36) have
 been detd. by x-ray diffractometry. The complexes described in this work
 are active in the MAO-mediated polymn. of ethylene.

08/01/2002

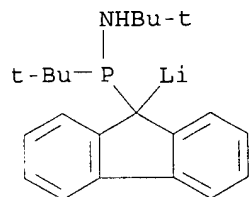
Serial No.:09/812,647

IT 440352-13-6P 440352-14-7P 440352-19-2P
440352-20-5P 440352-21-6P
RL: SPN (Synthetic preparation); PREP (Preparation))
RN 440352-13-6 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED



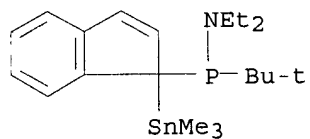
● Li

RN 440352-14-7 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED

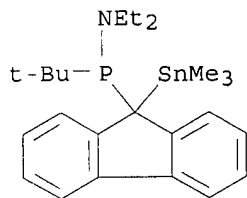


● Li

RN 440352-19-2 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED



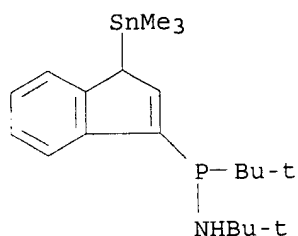
RN 440352-20-5 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED



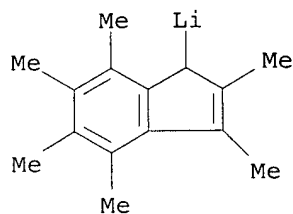
08/01/2002

Serial No.:09/812,647

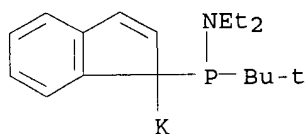
RN 440352-21-6 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED



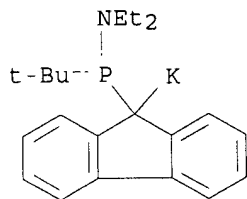
IT 440352-32-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(phosphination of)
RN 440352-32-9 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED

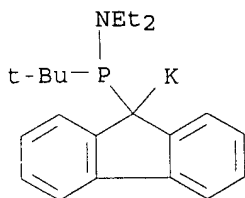


IT 405226-69-9P 405226-70-2P 440352-15-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and stannylation of)
RN 405226-69-9 HCAPLUS
CN Potassium, [1-[(diethylamino)(1,1-dimethylethyl)phosphino]-1H-inden-1-yl]-
(9CI) (CA INDEX NAME)

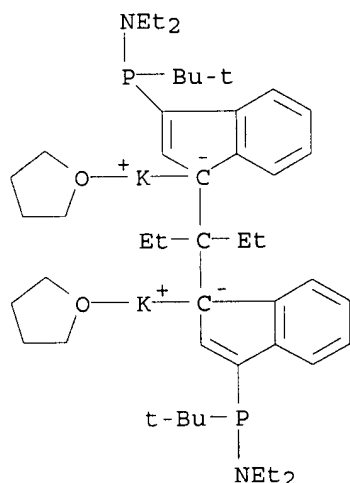


RN 405226-70-2 HCAPLUS
CN Potassium, [9-[(diethylamino)(1,1-dimethylethyl)phosphino]-9H-fluoren-9-yl]- (9CI) (CA INDEX NAME)





RN 440352-15-8 HCAPLUS
 CN Potassium, [μ -[(1-ethylpropylidene)bis[3-[(diethylamino)(1,1-dimethylethyl)phosphino]-1H-inden-1-ylidene]]]bis(tetrahydrofuran)di-(9CI) (CA INDEX NAME)



RE.CNT 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2002 ACS
 AN 2002:207066 HCAPLUS
 DN 136:385784
 TI Anionic Cyclization of a Cross-Conjugated Enediyne
 AU Eshdat, Lior; Berger, Harald; Hopf, Henning; Rabinovitz, Mordecai
 CS Department of Organic Chemistry, The Hebrew University of Jerusalem, Jerusalem, 91904, Israel
 SO Journal of the American Chemical Society (2002), 124(15), 3822-3823
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 AB Cross-conjugated enediynes cannot follow the Bergman cycloaromatization as it involves a methylenediyne moiety with only five π e-, insufficient for aromatization. Under reductive conditions the cyclization is made feasible by generating a product with a Huckel no. of π electrons. This principle is illustrated and the authors demonstrate for the first time an anionic cyclization of a cross-conjugated enediyne that results in formation of a five-membered ring. 9-(3-Phenyl-1-phenylethynylprop-2-ynylidene)-9H-fluorene was reduced by potassium to yield the dianion of 9-(3,4-diphenylcyclopenta-2,4-dienylidene)-9H-fluorene, which contains a

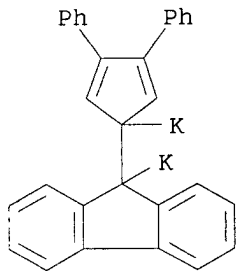
cyclopentadienyl fragment, and oxidn. with iodine yielded the unstable corresponding fulvalene.

IT 426258-19-7P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(proton and carbon-13 NMR study on anionic cyclization of cross-conjugated enediyne)

RN 426258-19-7 HCAPLUS

CN Potassium, [mu. - [(3,4-diphenyl-2,4-cyclopentadien-1-ylidene)-9H-fluoren-9-ylidene]]di- (9CI) (CA INDEX NAME)



RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2002 ACS

AN 2002:185852 HCAPLUS

DN 136:386221

TI Organic Syntheses via Transition Metal Complexes. 116. Carbocyclic Four-, Five-, and Six-Membered Rings by Condensation of (Alkyl,ethoxy)carbene Complexes (M = W, Cr) with .alpha.,.beta.-Unsaturated Tertiary Acid Amides
AU Aumann, Rudolf; Vogt, Dominik; Fu, Xiaolin; Froehlich, Roland; Schwab, Pia
CS Organisch-Chemisches Institut, Universitaet Muenster, Muenster, D-48149, Germany

SO Organometallics (2002), 21(8), 1637-1645

CODEN: ORGND7; ISSN: 0276-7333

PB American Chemical Society

DT Journal

LA English

AB 4-Amino-1-tungsta-1,3,5-hexatrienes (CO)5W:C(OEt)CH:C(NR2)CH:CHPh (2E,4E)-2 and (cyclohexan-4-on-1-yl)carbene W complexes 6 (e.g. I, NR2 = pyrrolidino) were obtained by condensation of (ethoxy,methyl)carbene W complex (OC)5W:C(OEt)CH3 1a with .alpha.,.beta.-unsatd. tertiary acid amides PhCH:CHC(:O)NR2 7 in the presence of POCl3/Et3N and (COCl)2/Et3N, resp. Compds. 2 underwent a .pi.-cyclization to zwitterionic .eta.1-cyclopentadiene complexes 3 (shown as II; R2N = Me2N, pyrrolidino). Condensation of (prim-alkyl,ethoxy)carbene complexes (CO)5M:C(OEt)CH2R1 1 (M = W, Cr; R1 = 2,4,6-cycloheptatrienyl, Pr) with compds. 7 afforded (cyclobutenyl)carbene complexes 9 (e.g. III, R1 = 2,4,6-cycloheptatrienyl). The crystal and mol. structures of (3E) - (CO)5W:C(OEt)CH:C(pyrrolidino)CH:CHPh, II and III were detd. by x-ray crystallog.

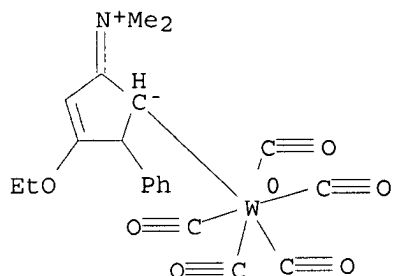
IT 425620-10-6P 425620-12-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(diastereoselective formation from ethoxyalkylidene complex and .alpha.,.beta.-unsatd. tertiary acid amide)

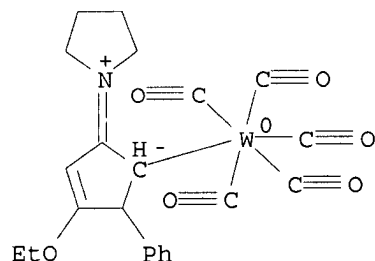
08/01/2002

Serial No.:09/812,647

RN 425620-10-6 HCAPLUS
CN Tungsten, pentacarbonyl[5-(dimethyliminio)-3-ethoxy-2-phenyl-3-cyclopenten-1-yl]-, (OC-6-21)- (9CI) (CA INDEX NAME)



RN 425620-12-8 HCAPLUS
CN Tungsten, pentacarbonyl(3-ethoxy-2-phenyl-5-pyrrolidinium-1-ylidene-3-cyclopenten-1-yl)-, (OC-6-21)- (9CI) (CA INDEX NAME)



RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2002 ACS
AN 2002:182586 HCAPLUS
DN 137:6247
TI Synthesis and crystal structure of cyclopentylindene rare earth complex
(C₅H₉C₉H₆)₃SmCl-Li+(THF)₄
AU Cui, Dong-mei; Tang, Tao; Cheng, Jian-hua; Hu, Ning-hai; Chen, Wen-qi;
Huang, Bao-tong
CS State Key Lab. of Polymer Physics and Chemistry, Changchun Institute of
Applied Chemistry, Chinese Academy of Sciences, Changchun, 130022, Peop.
Rep. China
SO Gaodeng Xuexiao Huaxue Xuebao (2002), 23(2), 188-190
CODEN: KTHPDM; ISSN: 0251-0790
PB Gaodeng Jiaoyu Chubanshe
DT Journal
LA Chinese
AB Rare earth complex (C₅H₉C₉H₆)₃SmCl-Li+(THF)₄ (I) was synthesized in 68%
yield by treating anhyd. SmCl₃ with two equiv C₅H₉C₉H₆Li in THF. The
intermediate was prepd. in 39% yield by treating indene with metallic Li
in THF and then with bromocyclopentane. From mixed THF and hexane
solvent, red single crystals of I were obtained. The crystal belongs to a
cubic system, space group P213 with a = b = c = 1.754 0(2) nm, .alpha. =
.beta. = .gamma. = 90.degree., V = 5.396 4(11) nm³, Z = 4. The
ten-coordinated Sm atom is bonded to three cyclopentylindenyl rings and a

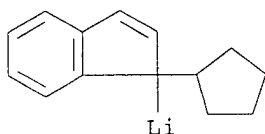
Cl atom to form the anionic part of the title complex, ring centroids and the Cl atom form a distorted tetrahedron around Sm. In the cationic part, a Li atom coordinates to four O atoms of THF mols. to form a normal tetrahedron. The Sm-C (within the same ring) distance varies from 0.268 to 0.299 nm.

IT 433330-95-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with samarium trichloride in THF)

RN 433330-95-1 HCAPLUS

CN Lithium, (1-cyclopentyl-1H-inden-1-yl)- (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2002 ACS

AN 2002:123875 HCAPLUS

DN 136:309985

TI Synthesis, Structural Characterization, and Reactivity of Organolanthanide Complexes Derived from a New, Versatile Boron-Bridged Ligand, $i\text{Pr}_2\text{NB}(\text{C}_9\text{H}_7)(\text{C}_2\text{B}_{10}\text{H}_{11})$

AU Zi, Guofu; Li, Hung-Wing; Xie, Zuowei

CS Department of Chemistry, Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, Peop. Rep. China

SO Organometallics (2002), 21(6), 1136-1145

CODEN: ORGND7; ISSN: 0276-7333

PB American Chemical Society

DT Journal

LA English

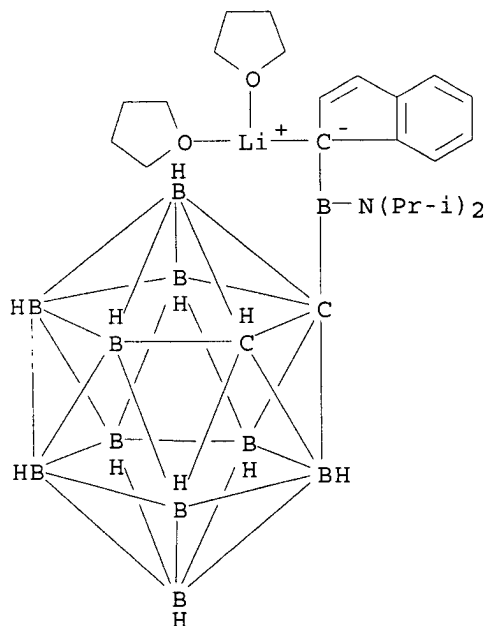
OS CASREACT 136:309985

AB New boron-bridged ligands incorporating both indenyl and carboranyl moieties have been prepd. Reaction of $i\text{Pr}_2\text{NB}(\text{C}_9\text{H}_7)\text{Cl}$ with 1 equiv. of $\text{LiC}_2\text{B}_{10}\text{H}_{10}$ gave, after treatment with 1 equiv. of $n\text{-BuLi}$, the dilithium salt $[i\text{Pr}_2\text{NB}(\text{C}_9\text{H}_6)(\text{C}_2\text{B}_{10}\text{H}_{10})]\text{Li}_2(\text{OEt})_2$ (1), which was conveniently converted into its neutral counterpart $i\text{Pr}_2\text{NB}(\text{C}_9\text{H}_7)(\text{C}_2\text{B}_{10}\text{H}_{11})$ (2) via reaction with excess C_5H_6 . Mixing 1 and 2 in a 1:1 molar ratio quant. afforded the monolithium salt $[i\text{Pr}_2\text{NB}(\text{C}_9\text{H}_6)(\text{C}_2\text{B}_{10}\text{H}_{11})]\text{Li}(\text{THF})_2$ (3). Treatment of LnI_2 with 1 equiv. of 1 generated the trivalent organolanthanide complexes $\text{meso}-[\{\text{.eta.5:}.\text{sigma.}-i\text{Pr}_2\text{NB}(\text{C}_9\text{H}_6)(\text{C}_2\text{B}_{10}\text{H}_{10})\}_2\text{Ln}][\text{Li}(\text{S})_n]$ ($\text{Ln} = \text{Sm}, \text{Yb}$; $\text{S} = \text{THF}$, $n = 4$; $\text{S} = \text{DME}$, $n = 3$), which was also prepd. in a much higher yield by reaction of LnI_2 with 1 equiv. of 1 followed by treatment with 1 equiv. of 3. Both inter- and intramol. electron-transfer pathways are proposed for these reactions. Reaction of LnCl_3 with 1 or 2 equiv. of 1 gave the same ionic complexes $\text{meso}-[\{\text{.eta.5:}.\text{sigma.}-i\text{Pr}_2\text{NB}(\text{C}_9\text{H}_6)(\text{C}_2\text{B}_{10}\text{H}_{10})\}_2\text{Ln}][\text{Li}(\text{S})_n]$ ($\text{Ln} = \text{Nd}, \text{Y}, \text{Yb}$; $\text{S} = \text{THF}$, $n = 4$; $\text{S} = \text{DME}$, $n = 3$). Silylamine elimination reactions of 2 and $\text{Ln}[\text{N}(\text{SiHMe}_2)_2]_3(\text{THF})_2$ resulted in clear formation of $[\text{.eta.5:}.\text{sigma.}-i\text{Pr}_2\text{NB}(\text{C}_9\text{H}_6)(\text{C}_2\text{B}_{10}\text{H}_{10})]\text{LnN}(\text{SiHMe}_2)_2(\text{THF})_2$ ($\text{Ln} = \text{Nd}$ (8), Er (9), Y (10)). Treatment of 8 with Me_3NHCl or Me_3SiCl led to the isolation of 2 and $\text{NdCl}_3(\text{DME})_2$, resp. The new complexes were fully characterized by various spectroscopic data and element analyses. Some were further confirmed by single-crystal x-ray analyses. Complex 8 is an active catalyst for the polymn. of Me methacrylate (MMA) in toluene, affording

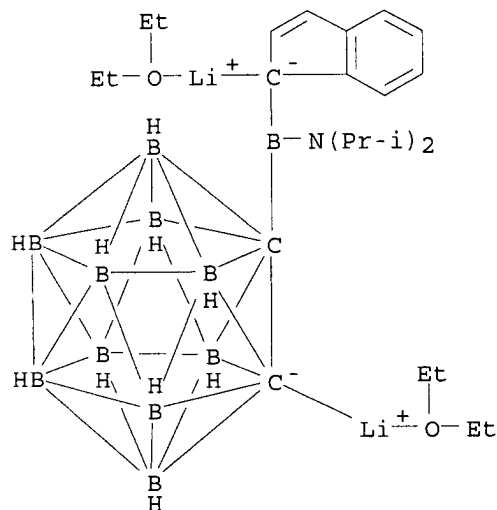
08/01/2002

Serial No.:09/812,647

syn-rich poly(MMA)s.
IT **412003-69-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 412003-69-1 HCAPLUS
CN Lithium, [1-[[bis(1-methylethyl)amino]-1,2-dicarbadoecaboran(12)-1-ylboryl]-1H-inden-1-yl]bis(tetrahydrofuran)- (9CI) (CA INDEX NAME)



IT **412003-67-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(synthesis, structural characterization, and reactivity of
organolanthanide complexes derived carboranyl indenyl aminoborane as
new, versatile boron-bridged ligand)
RN 412003-67-9 HCAPLUS
CN Lithium, [μ -[1,2-dicarbadoecaborane(12)-1,2-diyl{[bis(1-
methylethyl)amino]borylene}-1H-inden-1-ylidene]]bis[1,1'-oxybis[ethane]]di-
(9CI) (CA INDEX NAME)



RE.CNT 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2002 ACS
AN 2002:90667 HCAPLUS
DN 136:311018
TI Isotactic-Hemiisotactic Polypropylene from C1-Symmetric ansa-Metallocene Catalysts: A New Strategy for the Synthesis of Elastomeric Polypropylene
AU Miller, Stephen A.; Bercaw, John E.
CS Arnold and Mabel Beckman Laboratories of Chemical Synthesis, California Institute of Technology, Pasadena, CA, 91125, USA
SO Organometallics (2002), 21(5), 934-945
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
AB Control of isotactic-hemiisotactic alignment, a polypropylene microstructure in which every other stereocenter is of the same configuration and the intervening stereocenters tend to align with their neighbors, was achieved by R substituent selection in the ansa-metallocene catalyst system $R'2C(\eta^5-3-R-C5H3)(\eta^5-C13H8)MCl2$ -MAO (M = Zr, Hf; R' = Me, Ph; R = Me, 2-adamantyl, endo-2-norbornyl, 3,3,5,5-tetramethylcyclohexyl, $\eta^5-3-R-C5H3 = \eta^5-3-t-Bu-4-Me-C5H2$; $\eta^5-C13H8 = fluorenyl$; MAO = methylaluminoxane). For R = 2-adamantyl, R' = Ph, and M = Zr (4), α , a parameter equal to the m diad fraction, is ≈ 0.58 , with $M_n = 204,000-463,000$, and the isotactic-hemiisotactic polypropylene obtained is elastomeric. Typical elongations are 7-14 times the original length, and the residual elongation following a 200% strain is 1.5-9.3%. The elastomeric properties are rationalized by the statistical existence of isotactic stereoblocks among otherwise amorphous hemiisotactic connecting segments. A two-parameter (α and M_n) statistical model was derived which calcs. the isotactic block length distribution and the percent crystallinity, assuming isotactic blocks of 21 monomer units and longer participate in crystallites. The best elastomers have a calcd. percent crystallinity at 1.50-4.45% (α 0.557-0.630). Single crystal x-ray structure detns. are reported for 4 as its benzene solvates.

IT 408540-69-2P 408540-71-6P 408540-74-9P
408540-77-2P 408540-79-4P 408540-81-8P

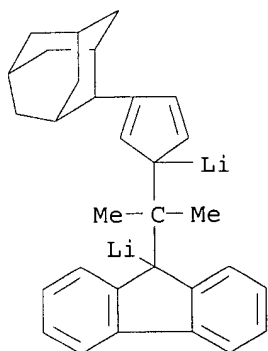
08/01/2002

Serial No.:09/812,647

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. of isotactic-hemiisotactic polypropylene using C1-sym.
ansa-metallocene catalysts)

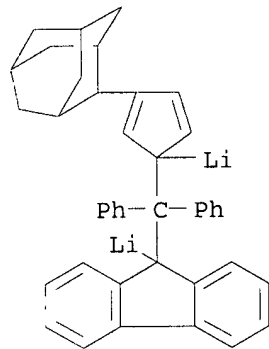
RN 408540-69-2 HCAPLUS

CN Lithium, [.mu.-[9H-fluoren-9-ylidene(1-methylethylidene)(3-
tricyclo[3.3.1.1^{3,7}]dec-2-yl-2,4-cyclopentadien-1-ylidene)]]di- (9CI) (CA
INDEX NAME)



RN 408540-71-6 HCAPLUS

CN Lithium, [.mu.-[9H-fluoren-9-ylidene(diphenylmethylene)(3-
tricyclo[3.3.1.1^{3,7}]dec-2-yl-2,4-cyclopentadien-1-ylidene)]]di- (9CI) (CA
INDEX NAME)



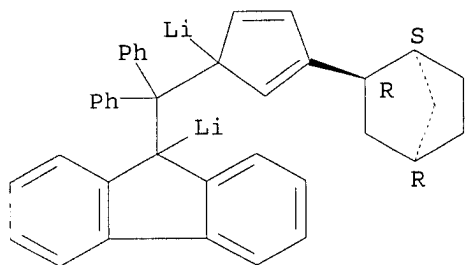
RN 408540-74-9 HCAPLUS

CN Lithium, [.mu.-[rel-[3-(1R,2S,4S)-bicyclo[2.2.1]hept-2-yl-2,4-
cyclopentadien-1-ylidene](diphenylmethylene)-9H-fluoren-9-ylidene]]]di-
(9CI) (CA INDEX NAME)

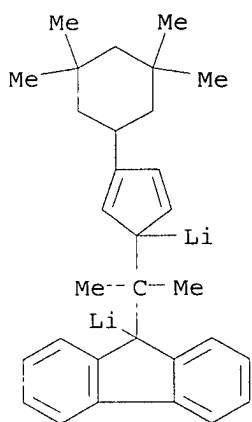
Relative stereochemistry.

08/01/2002

Serial No.:09/812,647

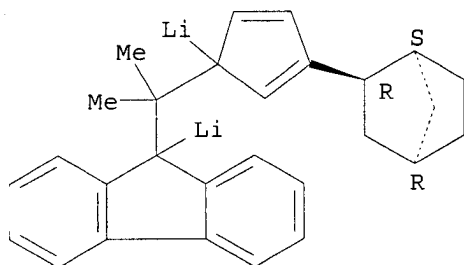


RN 408540-77-2 HCAPLUS
CN Lithium, [.mu.-[9H-fluoren-9-ylidene(1-methylethylidene)[3-(3,3,5,5-tetramethylcyclohexyl)-2,4-cyclopentadien-1-ylidene]]di- (9CI) (CA INDEX NAME)

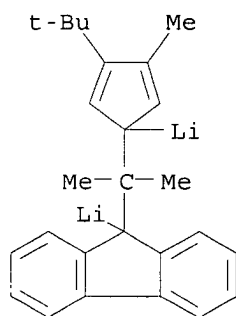


RN 408540-79-4 HCAPLUS
CN Lithium, [.mu.-[rel-[3-(1R,2S,4S)-bicyclo[2.2.1]hept-2-yl-2,4-cyclopentadien-1-ylidene](1-methylethylidene)-9H-fluoren-9-ylidene]]di- (9CI) (CA INDEX NAME)

Relative stereochemistry.

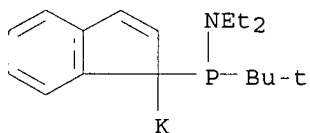


RN 408540-81-8 HCAPLUS
CN Lithium, [.mu.-[[3-(1,1-dimethylethyl)-4-methyl-2,4-cyclopentadien-1-ylidene](1-methylethylidene)-9H-fluoren-9-ylidene]]di- (9CI) (CA INDEX NAME)



RE.CNT 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

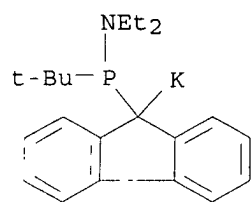
L5 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2002 ACS
AN 2001:791501 HCAPLUS
DN 136:263523
TI Alkylaminophosphanyl substituted half-sandwich complexes of vanadium(III) and chromium(III): preparation and reactivity in ethylene polymerisation
AU Kotov, Vasily V.; Avtomonov, Evgeni V.; Sundermeyer, Jorg; Aitola, Erkki; Repo, Timo; Lemenovskii, Dmitry A.
CS Department of Chemistry, Lomonosov Moscow State University, Vorobevy Gory, RUS-119899, Russia
SO Journal of Organometallic Chemistry (2001), 640(1-2), 21-28
CODEN: JORCAI; ISSN: 0022-328X
PB Elsevier Science S.A.
DT Journal
LA English
AB [CpR(RPNet₂)]M (CpR = t-BuC₅H₃, C₅(CH₃)₄, indenyl, fluorenyl; M = Li, K) smoothly reacted with VCl₃(Me₃P)₂ and CrCl₃(THF)₃ giving paramagnetic complexes [CpR(R₁PNet₂)]MCl₂ (M = V(Me₃P)₂, Cr). After reaction with MAO these complexes were active in the polymn. of ethylene yielding highly cryst., high-d. products of high mol. wt. (Mw ranging from 100,000 to 4.5.times.10⁶ g mol⁻¹, 20 .ltoreq. Tp .ltoreq. 100 .degree.C). Polymn. with chromium complexes led to the formation of polyethylenes with broad mol. wt. distribution.
IT 405226-69-9 405226-70-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(in prepn. of alkylaminophosphanyl substituted half-sandwich complexes of vanadium(III) and chromium(III) catalysts for polymn. of ethylene)
RN 405226-69-9 HCAPLUS
CN Potassium, [1-[(diethylamino)(1,1-dimethylethyl)phosphino]-1H-inden-1-yl]-(9CI) (CA INDEX NAME)



RN 405226-70-2 HCAPLUS
CN Potassium, [9-[(diethylamino)(1,1-dimethylethyl)phosphino]-9H-fluoren-9-yl]-(9CI) (CA INDEX NAME)

08/01/2002

Serial No.:09/812,647



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L4: Entry 1 of 2

File: DWPI

Oct 25, 2001

DERWENT-ACC-NO: 2002-065894

DERWENT-WEEK: 200209

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TITLE: Molecular dipolar rotor for use in microelectronics, comprises a base, an axle connected to the base and orientated substantially perpendicular to the base, and a rotor portion having an electric dipole moment

INVENTOR: MAGNERA, T F; MICHL, J ; PRICE, J C

PATENT-ASSIGNEE:

ASSIGNEE

CODE

MAGNERA T F

MAGNI

MICHL J

MICHI

PRICE J C

PRICI

PRIORITY-DATA: 2000US-190648P (March 20, 2000), 2001US-0812647 (March 20, 2001)

PATENT-FAMILY:

PUB-NO

PUB-DATE

LANGUAGE

PAGES

MAIN-IPC

US 2001033937 A1

October 25, 2001

024

C07F007/12

APPLICATION-DATA:

PUB-NO

APPL-DATE

APPL-NO

DESCRIPTOR

US2001033937A1

March 20, 2000

2000US-190648P

Provisional

US2001033937A1

March 20, 2001

2001US-0812647

INT-CL (IPC): B32 B 2/04; C07 F 7/12

RELATED-ACC-NO: 2001-440620

ABSTRACTED-PUB-NO: US2001033937A

BASIC-ABSTRACT:

NOVELTY - Providing a molecular dipolar rotor which will rotate under application of a force for use in functional devices.

DETAILED DESCRIPTION - A molecular dipolar rotor comprises:

(i) a base;

(ii) an axle connected to the base and orientated substantially perpendicular to the base; and

(iii) a rotor portion having an electric dipole moment.

INDEPENDENT CLAIMS are also included for:

(1) a surface-mounted array of dipolar rotors comprising the claimed dipolar rotors where the base is covalently attached to the surface;

(2) a device comprising the claimed dipolar rotor and an excitation source that can induce movement of the rotor portion of the dipolar rotor;

(3) molecular dipolar rotors of formulae (I) - (IV) where the chlorine attached to the silicon act as leaving groups upon reaction with a surface.

M = transition metal;

Z = -Hg-S-Z';

Z' = -(CH₂)_nSi(OR)₃;

n = 0-15;

R = (un)substituted alkyl, where OR act as a leaving group upon reaction with a surface;

Y = polar or charged group; and

X = polar or charged group.

USE - Used in micromechanics, molecular electronics, statistical physics and material science.

ADVANTAGE - The dipolar rotor will rotate under application of a force.

DESCRIPTION OF DRAWING(S) - Figure 4 shows an example of dipole rotors mounted on quartz.

CHOSEN-DRAWING: Dwg.4/15

TITLE-TERMS: MOLECULAR DIPOLE ROTOR MICROELECTRONIC COMPRISE BASE AXLE
CONNECT BASE ORIENT SUBSTANTIAL PERPENDICULAR BASE ROTOR PORTION
ELECTRIC DIPOLE MOMENT

DERWENT-CLASS: E11 E12 L03 P73 U12

CPI-CODES: E05-E02D; E05-L; E05-M; E05-N; L03-D01;

EPI-CODES: U12-B03F;

CHEMICAL-CODES:

Chemical Indexing M3 *01*

Fragmentation Code
B414 B720 B741 B752 B831 C017 H6 H602 H681 M280
M311 M321 M342 M361 M391 M411 M510 M520 M530 M540
M620 M781 M904 M905 Q454 R043
Specific Compounds
A5RPRK A5RPRU

Chemical Indexing M3 *02*

Fragmentation Code
B514 B720 B741 B752 B831 C017 G018 G100 H5 H542
H7 H731 H8 K0 L1 L143 L199 M210 M211 M272
M282 M312 M321 M332 M342 M351 M391 M411 M510 M520
M531 M540 M781 M904 M905 Q454 R043
Specific Compounds
A5RPTK A5RPTU

Chemical Indexing M3 *03*

Fragmentation Code
B414 B720 B741 B752 B831 C017 H6 H602 H681 H7
H731 M280 M313 M321 M332 M342 M361 M391 M411 M510
M520 M530 M540 M781 M904 M905 Q454 R043
Specific Compounds
A5RPWK A5RPWU

Chemical Indexing M3 *04*

Fragmentation Code
A400 A500 A600 A680 A923 A960 B514 B713 B720 B721
B741 B831 G015 G019 G037 G039 G113 G541 G551 H498
M1 M113 M119 M126 M144 M210 M211 M212 M213 M214
M215 M216 M220 M221 M222 M223 M224 M225 M226 M231
M232 M233 M272 M283 M311 M312 M313 M314 M315 M316
M320 M321 M331 M332 M340 M342 M361 M391 M411 M510
M520 M533 M542 M630 M650 M781 M904 M905 Q454 R043
Markush Compounds
200052-34801-K 200052-34801-U

SECONDARY-ACC-NO:

CPI Secondary Accession Numbers: C2002-019495

Non-CPI Secondary Accession Numbers: N2002-048969